easypipe Documentation

Release 1.4.2

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You can also grab a hardcopy of the easYPipe documentation in PDF

CHAPTER

ONE

GETTING STARTED (LINUX)

1.1 Check your python version

First, open a terminal.

easYPipe needs at least Python 3.6.

You may already have Python installed – you can check which version by doing:

```
$ python --version
```

If the version is < 3.0, do:

```
$ python3 --version
```

If that fails or Python 3 version is <3.6, install a version of Python >= 3.6 using the package manager of your distribution. For example for Ubuntu 16.10 or newer:

Installing add-apt-repository (if add-apt-repository command not found):

```
$ sudo apt update
$ sudo apt install software-properties-common
```

Then:

```
$ sudo add-apt-repository ppa:deadsnakes/ppa
$ sudo apt update
$ sudo apt-get install python3.6
```

If you've updated you Python version from 3.5 to 3.6, you can change default Python 3 to Python 3.6:

```
$ update-alternatives --install /usr/bin/python3 python3 /usr/bin/python3.5 1
$ update-alternatives --install /usr/bin/python3 python3 /usr/bin/python3.6 2
```

Check that Python 3 has been correctly installed:

```
$ python3 --version
Python 3.6
```

To swap between versions of Python, run the following:

```
$ update-alternatives --config python3
```

1.2 Check if pip is installed

pip is a package management tool for Python.

Check if pip3 is installed:

```
$ which pip3
```

If that fails, install pip3 using the package manager of your distribution. For example for Ubuntu:

```
$ sudo apt-get install python3-pip
```

Check if pip3 is linked to Python >= 3.6:

```
$ pip3 --version
pip 21.0.1 from /home/username/.local/lib/python3.6/site-packages/pip (python 3.6)
```

If it's not the case, you can try:

```
$ wget https://bootstrap.pypa.io/get-pip.py
$ sudo python3 get-pip.py
then check:
$ pip3 --version
```

1.3 Software requirements

easYPipe is a pipeline that requires other software.

1.3.1 Phenix

You need Phenix[1] installed and to modify PHENIX_PATH value in config.py file accordingly.

Example for PHENIX_PATH in config.py:

```
PHENIX_PATH = "/usr/local/phenix-1.18.2-3874/"
```

1.3.2 Open Babel

Open Babel[2] is a chemical toolbox needed for ligands.

Example for BABEL_PATH in config.py:

```
BABEL_PATH =  "/usr/local/OPENBABEL/openbabel-2-4-1/build/bin/"
```

Important: paths to these software have to be modified in config.py file accordingly to your installation (see next step)

[1] https://www.phenix-online.org/
[2] http://openbabel.org/wiki/Main_Page

1.4 Download and install easypipe package

Download the zip archive that should look like easypipe-1.4.2.tar.gz.

Go where is the archive and unzip:

```
$ tar -xvzf easypipe-1.4.2.tar.gz
```

Go to folder easypipe-1.4.2:

```
$ cd easypipe-1.4.2
```

Modify (open in a text editor) **config.py** file (in easypipe-1.4.2 folder), in particular 'Software used by modules' part since nothing will work without links to *software*.

> **Warning:** **config.py** file modifications have to be done before installation !! If you want to modify it afterwards, just launch installation again.

Then install:

```
$ sudo python setup.py install # if your default python version is >=3.6
or
$ sudo python3 setup.py install # if your python3 version is >=3.6
or
$ sudo python3.6 setup.py install # if your python3 version is linked to python3.5
```

If you've updated you Python version from 3.5 to 3.6, you may encountered some dependecies and conflict problems. Read carefully the error messages. These commands can help you:

```
$ sudo apt-get install libffi-dev

$ sudo pip3 uninstall PyNaCl
$ sudo pip3 install PyNaCl

$ sudo pip3 install setuptools_rust

$ cd /usr/lib/python3/dist-packages
$ sudo ln -s apt_pkg.cpython-{35m,36m}-x86_64-linux-gnu.so
```

1.5 Check easypipe installation

You can test if installation is successfull doing:

```
$ easypipe.py -h
```

If you get no error but the help message, easypipe installation is successfull.

If you've updated you Python version from 3.5 to 3.6, you may encountered the following error:

```
$ PermissionError: [Errno 13] Permission denied: '/usr/local/lib/python3.6/dist-
↪packages/easypipe-1.4.2-py3.6.egg/EGG-INFO/requires.txt'
```

In this case, this command should help:

```
$ cd /usr/local/lib/python3.6/dist-packages/easypipe-1.4.2-py3.6.egg/EGG-INFO/
$ sudo chmod a+r requires.txt
```

In the way, if you have 3.8 Python version (in Ubuntu 20.04 for example), you may encountered the following error:

```
$ PermissionError: [Errno 13] Permission denied: '/usr/local/lib/python3.8/dist-
↪packages/easypipe-1.4.2-py3.8.egg/EGG-INFO/requires.txt'
```

In this case, this command should help:

```
$ cd /usr/local/lib/python3.8/dist-packages/easypipe-1.4.2-py3.8.egg/EGG-INFO/
$ sudo chmod a+r requires.txt
```

1.6 Uninstall easypipe package

To uninstall easypipe package properly, do:

```
$ sudo pip3 uninstall easypipe
or
$ sudo python3 -m pip uninstall easypipe
or
$ sudo python3.6 -m pip uninstall easypipe
```

Note: 'pip3 freeze' lists the names of all python packages installed.

1.7 References

CHAPTER

TWO

GETTING STARTED (WINDOWS)

2.1 Check your python version

First, open a Command Prompt.

Note: To open Command Prompt, simply type 'cmd' in the search box of the Windows taskar.

easYPipe needs at least Python 3.6.

You may already have Python installed – you can check which version by doing:

```
C:\> python --version
or
C:\> py -V
```

If Python version is <3.6, install the latest Python 3 version. Download the latest python version Python downloads site. You can follow instructions here. But what you need is simply:

```
- Run the installer. You can do so by double-clicking python-<version>.exe in your␣
↪Downloads folder.
- !!!! Check the box next to "Add Python <version> to PATH." It's at the bottom of␣
↪the window.
- Install Now (customize installation not compulsory).
- Click Disable path length limit. This ensures that Python (and other apps) to use␣
↪paths more than 260 characters in length.
```

Check that Python 3 has been correctly installed:

```
C:\> python --version
Python 3.9

or

C:\> py -V
Python 3.9
```

2.2 Software requirements

easYPipe is a pipeline that requires other software.

2.2.1 Phenix

You need Phenix[1] installed and to modify PHENIX_PATH value in config.py file accordingly.

Example for PHENIX_PATH in config.py:

```
PHENIX_PATH = r"C:\Users\myname\Phenix\phenix-installer-1.19.1-4122-intel-windows-x86_
↪64"
```

2.2.2 Open Babel

Open Babel[2] is a chemical toolbox needed for ligands.

Install Open Babel GUI for Windows.

Example for BABEL_PATH in config.py:

```
BABEL_PATH = r"C:\Program Files\OpenBabel-3.1.1"
```

2.2.3 Advices

Important: paths to these software have to be modified in config.py file accordingly to your installation (see next step)

Tip: it might be wise to use LibreOffice[3] as many csv spreadsheets are generated by easYPipe and Excel does not handle the official csv format (i.e. comma-separated values) well for non-English speaking versions

2.3 Download and install easypipe package

Download the zip archive that should look like easypipe-1.4.2.tar.gz.

Go where is the archive and unzip:

```
C:\> tar -xvzf easypipe-1.4.2.tar.gz
```

Go to folder easypipe-1.4.2:

```
C:\> cd easypipe-1.4.2
```

Modify (open with a text editor like Notepad) **config.py** file (in easypipe-1.4.2 folder), in particular 'Software used by modules' part since nothing will work without links to *software*.

Warning: **config.py** file modifications have to be done before installation !! If you want to modify it afterwards, just launch installation again. Use a basic text editor and not a word processing software !

[1] https://www.phenix-online.org/
[2] http://openbabel.org/wiki/Main_Page
[3] https://www.libreoffice.org/

Then install:

```
C:\> python setup.py install
or
C:\> py setup.py install
```

2.4 Check easypipe installation

You can test if installation is successfull doing:

```
$ easypipe.py -h
```

If you get no error but the help message, easypipe installation is successfull.

Depending on your python version, you may encountered some dependecies and conflict problems. Read carefully the error messages.

In case of the following error:

```
$ cffi>=1.4.2 distribution was not found and is required by PyNaCl
```

This command should help:

```
$ py -m pip install cffi
```

2.5 Uninstall easypipe package

To uninstall easypipe package properly, do:

```
C:\>  pip uninstall easypipe
```

Note: 'py -m pip freeze' lists the names of all python packages installed.

2.6 References

CHAPTER

THREE

EASYGET

easYGet comes with *easYPipe*.

easYGet makes it possible to download all at once the mx 'PROCESSED_DATA' from a synchrotron for a given beamline (several dates possible) and a given acronym.

Downloaded processed datasets are organized by dataset folders, ready to launch easypipe.

For the moment, only works for data from Grenoble ESRF synchrotron.

3.1 easYGet usage

easyget.py [-h] [-s {ESRF}] [-l LOGIN] [[-m MX] [-b BEAMLINE] [-d DATES [DATES ...]] [-p PROTEIN] [-g GROUP]

optional arguments	description
-h, –help	show this help message and exit
-s {ESRF}, –synchrotron {ESRF}	which synchrotron? (default = ERSF)
-l LOGIN, –login LOGIN	synchrotron login (your personal SMIS login)
-m MX, –mx MX	name of mx proposalsynchrotron login (Example: 'mx—-')
-b BEAMLINE, –beamline BEAMLINE	name of the beamline
-d DATES [DATES ...], –dates DATES [DATES ...]	date of the run (format AAAAMMJJ) or list of dates for the same run (format AAAAMMJJ AAAAMMJJ)
-p PROTEIN, –protein PROTEIN	protein acronym or space if no acronym (manual collections)
-g GROUP, –group GROUP	group added via MxCube3 as a supplementary folder level before acronym

Information can be provided either in command line or in interactive mode in a terminal, or mix.

For example, you can simply run:

```
$ easyget.py
```

or:

```
$ easyget.py --login anna2502 --mx mx1000
```

or:

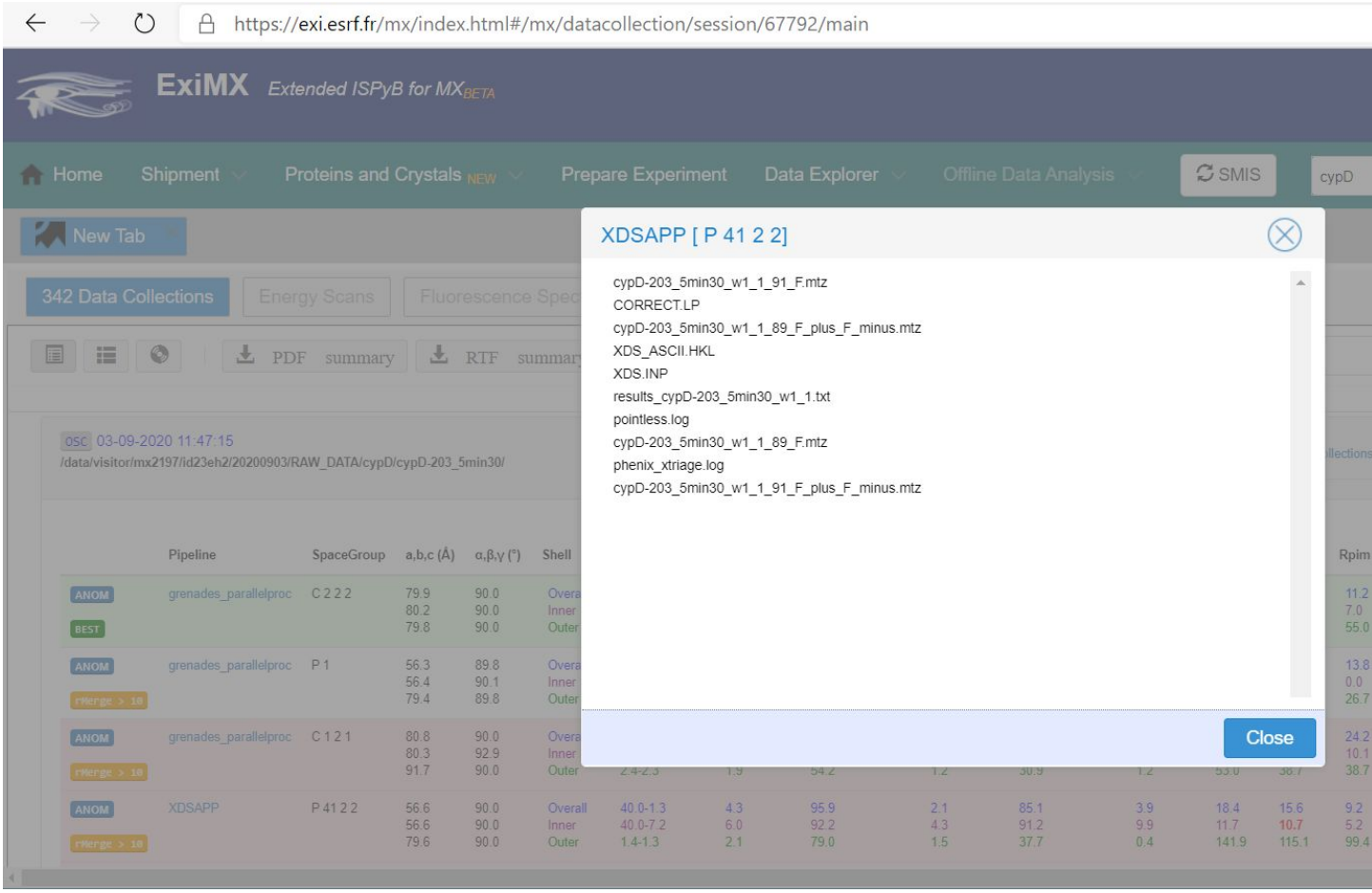
```
$ easyget.py --login anna2502 --mx mx1000 --protein myprot --beamline id30a1 --dates␣
↪20210131 20210201
```

other commands are possible . . .

Note: test also the day after each date given (useful for 24h experiments . . .)

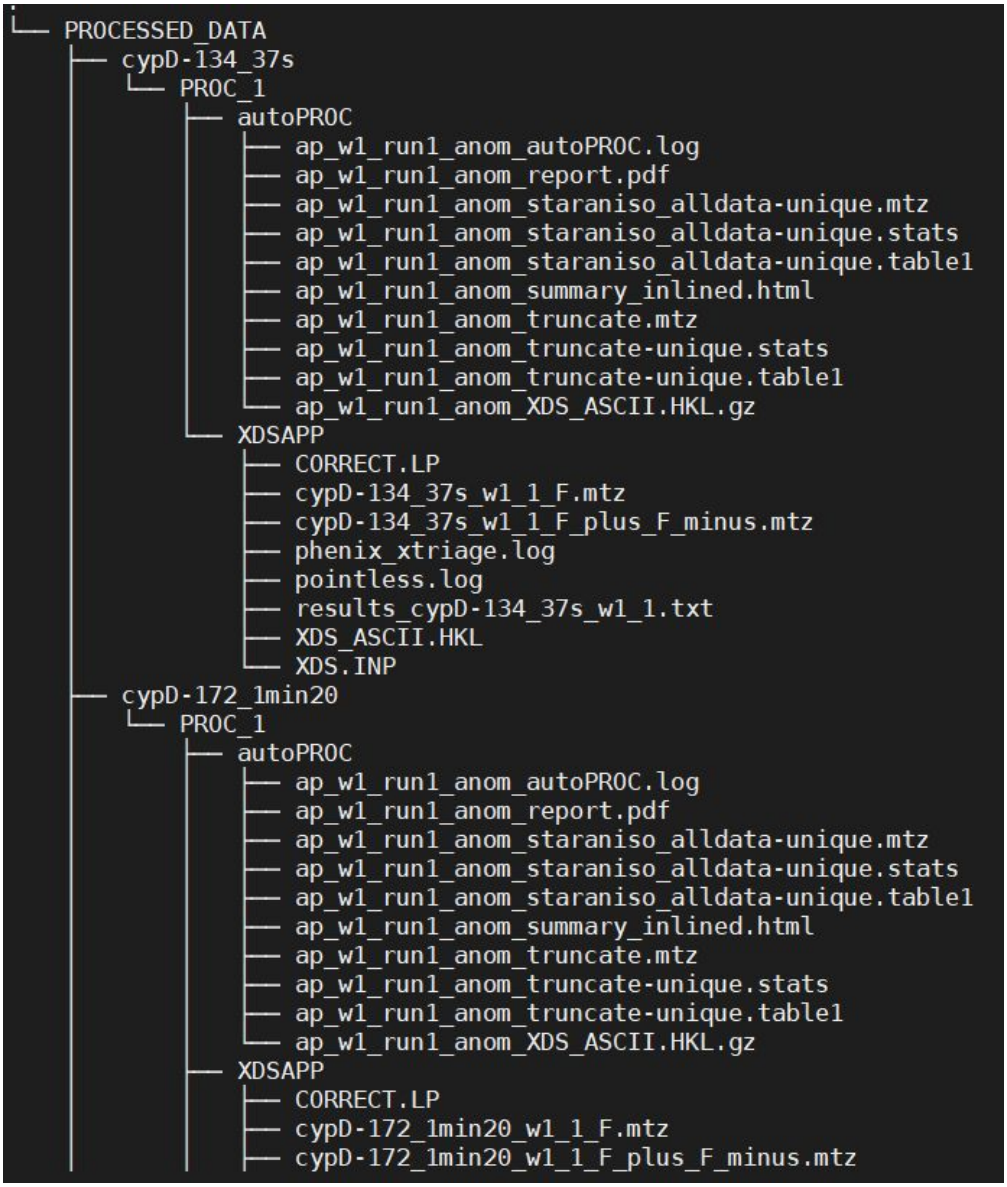
3.2 What does it do ?

Processed data @ESRF: for each crystal collected, several proccesses can succeed and for each a zip is available for download



All these processed data are copied this way by easYGet:

- **dataset folder for each dataset**
  - PROC_1, PROC_2, . . . if run 1, run 2 . . .
  - process sub-folder, with processed data for each process


PROCESSED_DATA
cypD-134_37s
PROC_1
autoPROC
ap_w1_run1_anom_autoPROC.log
ap_w1_run1_anom_report.pdf
ap_w1_run1_anom_staraniso_alldata-unique.mtz
ap_w1_run1_anom_staraniso_alldata-unique.stats
ap_w1_run1_anom_staraniso_alldata-unique.table1
ap_w1_run1_anom_summary_inlined.html
ap_w1_run1_anom_truncate.mtz
ap_w1_run1_anom_truncate-unique.stats
ap_w1_run1_anom_truncate-unique.table1
ap_w1_run1_anom_XDS_ASCII.HKL.gz
XDSAPP
CORRECT.LP
cypD-134_37s_w1_1_F.mtz
cypD-134_37s_w1_1_F_plus_F_minus.mtz
phenix_xtriage.log
pointless.log
results_cypD-134_37s_w1_1.txt
XDS_ASCII.HKL
XDS.INP
cypD-172_1min20
PROC_1
autoPROC
ap_w1_run1_anom_autoPROC.log
ap_w1_run1_anom_report.pdf
ap_w1_run1_anom_staraniso_alldata-unique.mtz
ap_w1_run1_anom_staraniso_alldata-unique.stats
ap_w1_run1_anom_staraniso_alldata-unique.table1
ap_w1_run1_anom_summary_inlined.html
ap_w1_run1_anom_truncate.mtz
ap_w1_run1_anom_truncate-unique.stats
ap_w1_run1_anom_truncate-unique.table1
ap_w1_run1_anom_XDS_ASCII.HKL.gz
XDSAPP
CORRECT.LP
cypD-172_1min20_w1_1_F.mtz
cypD-172_1min20_w1_1_F_plus_F_minus.mtz

CHAPTER

FOUR

EASYPIPE

easYPipe is a pipeline for the automatization of ligand and fragment X-Ray crystallographic screening.

easYPipe sequentially runs phenix.ligand_pipeline[1] on several datasets of a protein that has been screened with different ligands.

When ligand smiles are given, ligand can be placed automatically in each corresponding structure.

Results are gathered and organized in a 'RESULTS' directory, which facilitates future visualization, refinement and deposition. Corresponding relevant information is summarized in a csv file.

easYPipe is specially adapted for ligand or fragment screening in structure-based drug design projects.

See also:

easYGet that comes with easYPipe, for an automated download of processed data from synchrotron.

4.1 easYPipe usage

easypipe.py [-h] data {prep,reindex,ligands,launch,pandda} ...

arguments	description
data	folder with datasets in subfolders (mandatory)
-h, –help	show this help message and exit

Example:

```
$ easypipe.py PROCESSED_DATA -h
```

[1] https://www.phenix-online.org/documentation/reference/ligand_pipeline.html

subcommands	description
prep	prepare data: listing of mtz to treat with information
reindex	try to reindex mtz according to the space group of reference file
ligands	generate ligands files before launching with ligand search
launch	launch all the "phenix.ligand-pipeline" (after the preparation steps)
summary	compile the results of all the 'launch' execution in a single csv file
auto	run main easYPipe steps (prep, reindex, launch, summary) in automatic mode, but without ligand search
pandda	copy results from easypipe to a 'PANDDA' folder, as data ready to launch PanDDA

Example:

```
$ easypipe.py PROCESSED_DATA prep
```

You can have a look to the *quickstart guide*.

For a better experience, also read instructions for each subcommands.

4.1.1 References

CHAPTER

FIVE

EASYPIPE QUICKSTART GUIDE

5.1 1. Retrieve and organize your processed data

Note: You can retrieve your processed data from synchrotron using *easYGet*.

Processed data should be in datasets folders, all grouped in a folder. More information on how to organize your data *here*.

5.2 2. Prepare the data with 'prep'

The first step is intended to list mtz to be treated:

```
$ easypipe.py PROCESSED_DATA prep
```

where here 'PROCESSED_DATA' is the folder with your datasets.

Warning: For Windows users, $ is the Linux prompt that corresponds to C:> in Windows command prompt, and should not be written

Now, you can have a look at /easypipe/1a_prep/mtz_to_treat_ALL.csv file that lists mtz found in your processed data with information like resolution, completeness or space group.

For more details on this step see *here*.

5.3 3. Reindex if necessary with 'reindex'

If you see that some mtz should be in higher symmetry space group (in /easypipe/1a_prep/mtz_to_treat_ALL.csv file), then you can try to reindex.

Run:

```
$ easypipe.py PROCESSED_DATA reindex P41212
equivalent to:
$ easypipe.py PROCESSED_DATA reindex 92
```

For more details on this step see *here*.

5.4 4. Add ligands with 'ligands'

This step is necessary if you want Phenix to try to find and place ligands, or if you want to automatically generate the CIF and PDB of your ligands.

First, you have to fill in the fields <ligand name> and <ligand smiles> of /1c_ligands/ligands_for_datasets.csv file.

Then, run:

```
$ easypipe.py PROCESSED_DATA ligands easYPipe/1c_ligands/ligands_for_datasets_OK.csv
```

where here ligands_for_datasets_OK.csv is the name of your filled ligand csv file.

For more details on this step see *here*.

5.5 5. Process the data with 'launch'

Now you can run Phenix on your processed mtz.

5.5.1 Mode

Default mode, is 'fast' mode. This mode uses rigid body refinement and can be run to get a first result rapidly.

Example:

```
$ easypipe.py PROCESSED_DATA launch my_ref_folder
```

where my_ref_folder gather fasta file and pdb files for replacement, and cif file if there is a ligand in the model.

Warning: pdb files should include the row starting with 'CRYST1' containing information on space group

Now, have a look at your *results* in the corresponding 'RESULTS' csv file.

If some processes failed, they probably need longer calculations. You can try 'full' mode:

```
$ easypipe.py PROCESSED_DATA launch my_ref_folder --mode full
```

In case your protein changes its space group, with ligand for example, you can ask not to fix space group. As a result, all mtz could be treated even with 'bad' space group. The duration for this will be much longer. But you can only do it for some using simulation mode first (see above):

```
$ easypipe.py PROCESSED_DATA launch my_ref_folder --mode allsg
```

5.5.2 Ligand search

If you want LigandFit to place ligands, you first have to run 'ligand' subcommand (*see above*).

Then just add '–lig' option:

```
$  easypipe.py PROCESSED_DATA launch my_ref_folder --mode full --lig
```

The default cutoff for LigandFit to place a ligand is 0.7, but you can change it if you see that it is too high, with '–cclig' option:

```
$ easypipe.py PROCESSED_DATA launch my_ref_folder --mode full --lig --cclig 0.6
```

If several ligands are supposed to fix, you can ask for LigandFit to place more than one ligand, with '–nblig' option:

```
$ easypipe.py PROCESSED_DATA launch my_ref_folder --mode full --lig --cclig 0.6 --
↪nblig 5
```

5.5.3 Datasets to treat

Default behavior is to run phenix.ligand_pipeline on the mtz of best completeness for each dataset, you can start with it.

If there are failures in the treatment of 'best completeness' mtz, you can try to treat a higher number of mtz for each dataset.

You can first start by running on mtz from autoPROC process which is generally a good compromise between resolution and completeness:

```
$ easypipe.py PROCESSED_DATA launch my_ref_folder --mode full --lig --autoproc
```

Or you can run on the two first mtz of best completeness for each dataset:

```
$ easypipe.py PROCESSED_DATA launch my_ref_folder --mode full --lig --best 2
```

or more . . . :

```
$ easypipe.py PROCESSED_DATA launch my_ref_folder --mode full --lig --best 5
```

or on the whole processed mtz files:

```
$ easypipe.py PROCESSED_DATA launch my_ref_folder --mode full --lig --whole
```

If only some datasets are problematic, you can run in simulation mode first, modify the corresponding 'launch' csv file in /easYPipe/2_launch/ (replace 'yes' by 'no' in the 'to treat' column, for those not to process), then run again:

```
$ easypipe.py PROCESSED_DATA launch my_ref_folder --mode full --lig --whole --simulate
then, after modification of the 'launch' csv file:
$ easypipe.py PROCESSED_DATA launch my_ref_folder --mode full --lig --whole
```

Then, only selected mtz will be treated, reducing the duration of the treatment.

For more details on this step see *here*.

5.6 6. Compile results in a summary file

If you have run several times 'launch' subcommand, you will have several 'RESULT' csv files that you probably wish to compile and clean.

Then run:

```
$ easypipe.py PROCESSED_DATA summary
```

5.7 7. Automatic mode

This mode allows to run main easYPipe steps (prep, reindex, launch, summary) without any intervention. It could be a good starting point before running more 'launch' commands or ligand search.

Example:

```
$ easypipe.py PROCESSED_DATA auto my_ref_folder --best 2 --mode full
```

Note: Ligand search is not supported at this time in this mode.

For more details on this mode see *here*.

CHAPTER

SIX

EASYPIPE 'PREP'

Important: This step is a first mandatory step for the preparation of the data.

6.1 Usage

easypipe.py data prep [-h]

Example:

```
$ easypipe.py PROCESSED_DATA prep
```

6.2 How the data should be organized ?

The data folder (whatever it's name) must contain only datasets folders.

Within each dataset folder, the processed data can be organized in several ways:

- a mtz file directly in dataset folder
- a mtz file in a sub-folder, or in a sub-sub-folder ... of dataset folder
- several processes are possible for a dataset, provided that they are in different sub-folders
- if several mtz files are present in the same sub-folder, only one will be treated on the basis of templates (from ESRF EDNA processes)

```
- data folder
        - dataset1
                - file.mtz
                - other-file.log
                        :
        - dataset2
                - proc-folder
                        - file-direct.mtz
                        - other-file.txt
                        - other-file.csv
                                :
        - dataset3
                - PROC_1
                        -  autoPROC
                                - ap_cypD-122-2min_run1_anom_autoPROC.log
                                - ap_cypD-122-2min_run1_anom_report.pdf
                                - ap_cypD-122-2min_run1_anom_staraniso_alldata-unique.mtz
                                - ap_cypD-122-2min_run1_anom_staraniso_alldata-unique.stats
                                - ap_cypD-122-2min_run1_anom_staraniso_alldata-unique.table1
                                - ap_cypD-122-2min_run1_anom_summary_inlined.html
                                - ap_cypD-122-2min_run1_anom_truncate.mtz
                                - ap_cypD-122-2min_run1_anom_truncate-unique.stats
                                - ap_cypD-122-2min_run1_anom_truncate-unique.table1
                                - ap_cypD-122-2min_run1_anom_XDS_ASCII.HKL.gz
                        - another-process
                                :
                - PROC_2
                        :
```

Note: Data downloaded with *easYGet* are directly in the right tree organization.

6.3 What does it do ?

In an 'easYPipe' folder created at the place where it is executed, 'prep' copies each processed data mtz in a sub-folder of the dataset in this way:

- creation of an 'easYPipe' treatment directory where it is run
- creation of a subdirectory '0_processed_datasets' where all the datasets folder are created
- creation of a 'data' folder in each dataset folder and copy in this folder of processed mtz and log files
- if there are several mtz in a folder, search for 'EDNA' treatment template and selects the right mtz file

Then:

- launch of xtriage[1] for each mtz to get resolution, completeness, space group and cell parameters

[1] https://www.phenix-online.org/documentation/reference/xtriage.html

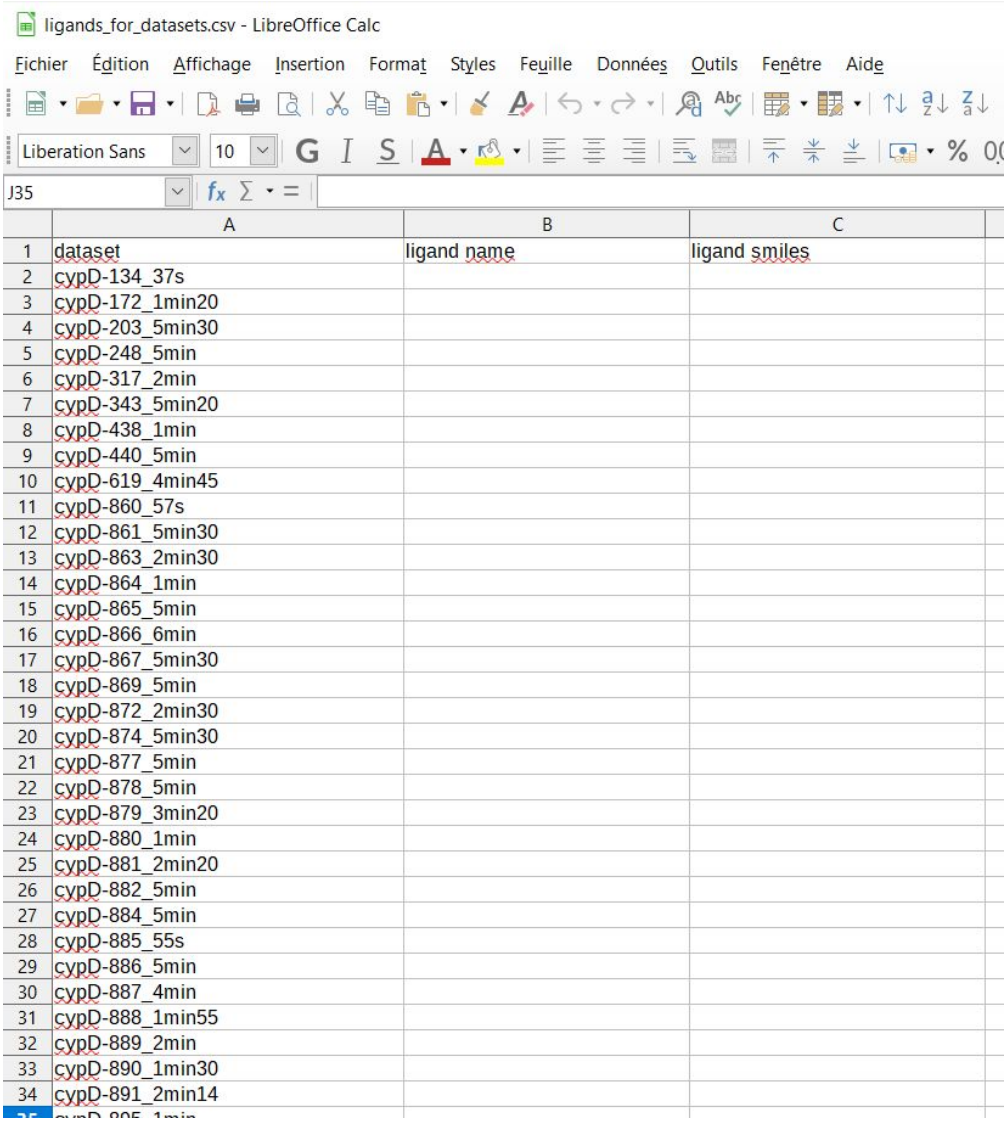
```
easYPipe/
├── 0_processed_datasets
    ├── cypD-134_37s
        ├── data
            ├── mtz001_PROC_1_autoPROC
                ├── ap_w1_run1_anom_autoPROC.log
                ├── ap_w1_run1_anom_truncate.mtz
                ├── ap_w1_run1_anom_XDS_ASCII.HKL.gz
                ├── xtriage_ap_w1_run1_anom_truncate.log
                ├── xtriage-verbose_labels.log
                └── xtriage-verbose.log
            └── mtz002_PROC_1_XDSAPP
                ├── CORRECT.LP
                ├── cypD-134_37s_w1_1_F_plus_F_minus.mtz
                ├── phenix_xtriage.log
                ├── pointless.log
                ├── XDS_ASCII.HKL
                ├── xtriage_cypD-134_37s_w1_1_F_plus_F_minus.log
                ├── xtriage-verbose_labels.log
                └── xtriage-verbose.log
        └── ligand
    ├── cypD-172_1min20
        ├── data
            ├── mtz001_PROC_1_autoPROC
                ├── ap_w1_run1_anom_autoPROC.log
                ├── ap_w1_run1_anom_truncate.mtz
                ├── ap_w1_run1_anom_XDS_ASCII.HKL.gz
                ├── xtriage_ap_w1_run1_anom_truncate.log
                ├── xtriage-verbose_labels.log
                └── xtriage-verbose.log
            ├── mtz002_PROC_1_XDSAPP
                ├── CORRECT.LP
                ├── cypD-172_1min20_w1_1_F_plus_F_minus.mtz
                ├── phenix_xtriage.log
                ├── pointless.log
                ├── XDS_ASCII.HKL
                ├── xtriage_cypD-172_1min20_w1_1_F_plus_F_minus.log
                ├── xtriage-verbose_labels.log
                └── xtriage-verbose.log
            └── mtz003_PROC_1_XIA2_DIALS
                ├── di_w1_run1_anom_AUTOMATIC_DEFAULT_aimless.log
```

- information on mtz files to be treated written in '/easypipe/1a_prep/mtz_to_treat_ALL.csv' file

	A	B	C	D	E	F	
1	dataset	mtz nb	process name	mtz file	resolution(A)	completeness(%)	spa
2	cypD-134_37s	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.31	97.98	P42
3	cypD-134_37s	mtz002	PROC_1_XDSAPP	cypD-134_37s_w1_1_F.mtz	1.64	42.53	P2
4	cypD-172_1min20	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	4.05	52.83	P1
5	cypD-172_1min20	mtz002	PROC_1_XDSAPP	cypD-172_1min20_w1_1_F.mtz	3.88	43.0	P1
6	cypD-172_1min20	mtz003	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free.mtz	3.08	71.63	P21
7	cypD-203_5min30	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.51	97.88	P42
8	cypD-203_5min30	mtz002	PROC_1_XDSAPP	cypD-203_5min30_w1_1_89_F.mtz	1.32	90.39	P42
9	cypD-203_5min30	mtz003	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free.mtz	1.67	83.63	C2
10	cypD-248_5min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.14	98.49	P41
11	cypD-248_5min	mtz002	PROC_1_EDNA_proc	ep_cypD-248_5min_w1_run1_anom_truncate.mtz	1.0	85.05	P41
12	cypD-248_5min	mtz003	PROC_1_XDSAPP	cypD-248_5min_w1_1_96_F.mtz	1.03	85.68	P43
13	cypD-248_5min	mtz004	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free.mtz	1.38	80.19	P2
14	cypD-317_2min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.14	98.9	P42
15	cypD-317_2min	mtz002	PROC_1_EDNA_proc	ep_cypD-317_2min_w1_run1_anom_truncate.mtz	1.07	95.13	P42
16	cypD-317_2min	mtz003	PROC_1_XDSAPP	cypD-317_2min_w1_1_92_F.mtz	1.06	90.43	P41
17	cypD-343_5min20	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.11	83.81	P41
18	cypD-343_5min20	mtz002	PROC_1_EDNA_proc	ep_cypD-343_5min20_w1_run1_anom_truncate.mtz	1.11	83.97	P41
19	cypD-343_5min20	mtz003	PROC_1_XDSAPP	cypD-343_5min20_w1_1_96_F.mtz	1.11	77.88	P43
20	cypD-343_5min20	mtz004	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free.mtz	1.44	83.17	C2
21	cypD-438_1min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.07	93.24	P42
22	cypD-438_1min	mtz002	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free.mtz	1.05	82.57	C22
23	cypD-440_5min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	2.7	57.25	P1
24	cypD-440_5min	mtz002	PROC_1_XDSAPP	cypD-440_5min_w1_1_92_F.mtz	1.62	96.57	P41
25	cypD-619_4min45	mtz001	PROC_1_EDNA_proc	ep_cypD-619_4min45_w1_run1_anom_truncate.mtz	1.96	90.86	P42
26	cypD-619_4min45	mtz002	PROC_1_XDSAPP	cypD-619_4min45_w1_1_F.mtz	1.96	90.86	P42
27	cypD-619_4min45	mtz003	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free.mtz	1.69	97.05	P42
28	cypD-860_57s	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	2.86	83.07	P42
29	cypD-860_57s	mtz002	PROC_1_EDNA_proc	ep_cypD-860_57s_w1_run1_anom_truncate.mtz	1.14	84.49	P41
30	cypD-860_57s	mtz003	PROC_1_XDSAPP	cypD-860_57s_w1_1_20_F.mtz	1.42	68.54	C22
31	cypD-860_57s	mtz004	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free.mtz	1.27	91.66	P22

-creation of a csv file '/easypipe/1c_ligands/ligands_for_datasets.csv' for future ligand generation with eLBOW[2]

[2] https://www.phenix-online.org/documentation/reference/elbow.html



	A	B	C
1	dataset	ligand name	ligand smiles
2	cypD-134_37s		
3	cypD-172_1min20		
4	cypD-203_5min30		
5	cypD-248_5min		
6	cypD-317_2min		
7	cypD-343_5min20		
8	cypD-438_1min		
9	cypD-440_5min		
10	cypD-619_4min45		
11	cypD-860_57s		
12	cypD-861_5min30		
13	cypD-863_2min30		
14	cypD-864_1min		
15	cypD-865_5min		
16	cypD-866_6min		
17	cypD-867_5min30		
18	cypD-869_5min		
19	cypD-872_2min30		
20	cypD-874_5min30		
21	cypD-877_5min		
22	cypD-878_5min		
23	cypD-879_3min20		
24	cypD-880_1min		
25	cypD-881_2min20		
26	cypD-882_5min		
27	cypD-884_5min		
28	cypD-885_55s		
29	cypD-886_5min		
30	cypD-887_4min		
31	cypD-888_1min55		
32	cypD-889_2min		
33	cypD-890_1min30		
34	cypD-891_2min14		

You have to fill 'ligand name' and 'ligand smiles' fields before running *'easYPipe ligands subcommand'*.

> **Caution:** Save the modified csv file somewhere else or with another name if you don't want to overwrite it in case you launch 'prep' sub-command again . . .

You can also run *'easYPipe reindex subcommand'* if some mtz should be in higher symmetry space group.

If you are not interested in ligand placement or reindexation, you can directly run *'easYPipe launch subcommand'*.

6.4 References

CHAPTER

SEVEN

EASYPIPE 'REINDEX'

This optional step is useful when several mtz should be in higher symmetry space group.

The program try to reindex according to the space group of the reference mtz.

Example: P422 can be re-indexed to P41212.

7.1 Usage

easypipe.py data reindex [-h] ref_mtz

arguments	description
-h, –help	show this help message and exit
sg_ref	space group of reference for reindexing (name or number)

Example:

```
$ easypipe.py PROCESSED_DATA reindex P41212
equivalent to:
$ easypipe.py PROCESSED_DATA reindex 92
```

7.2 What does it do ?

- try to reindex mtz file with reflection_file_converter[1] if space group is different from reference space group

[1] https://phenix-online.org/documentation/reference/reflection_file_tools.html

```
~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
~~                                  SUMMARY                                   ~~
~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
mtz candidates for reindexing (space group different from reference file): 93

cypD-134_37s/mtz001_PROC_1_autoPROC/ap_w1_run1_anom_truncate.mtz / P422
cypD-134_37s/mtz002_PROC_1_XDSAPP/cypD-134_37s_w1_1_F.mtz / P2
cypD-172_1min20/mtz001_PROC_1_autoPROC/ap_w1_run1_anom_truncate.mtz / P1
cypD-172_1min20/mtz002_PROC_1_XDSAPP/cypD-172_1min20_w1_1_F.mtz / P1
cypD-172_1min20/mtz003_PROC_1_XIA2_DIALS/di_w1_run1_anom_AUTOMATIC_DEFAULT_free.mtz / P21
cypD-203_5min30/mtz001_PROC_1_autoPROC/ap_w1_run1_anom_truncate.mtz / P422
cypD-203_5min30/mtz002_PROC_1_XDSAPP/cypD-203_5min30_w1_1_89_F.mtz / P422
cypD-203_5min30/mtz003_PROC_1_XIA2_DIALS/di_w1_run1_anom_AUTOMATIC_DEFAULT_free.mtz / C2
cypD-248_5min/mtz003_PROC_1_XDSAPP/cypD-248_5min_w1_1_96_F.mtz / P43212
cypD-248_5min/mtz004_PROC_1_XIA2_DIALS/di_w1_run1_anom_AUTOMATIC_DEFAULT_free.mtz / P2
cypD-317_2min/mtz001_PROC_1_autoPROC/ap_w1_run1_anom_truncate.mtz / P422
cypD-317_2min/mtz002_PROC_1_EDNA_proc/ep_cypD-317_2min_w1_run1_anom_truncate.mtz / P4212
cypD-343_5min20/mtz003_PROC_1_XDSAPP/cypD-343_5min20_w1_1_96_F.mtz / P43212
cypD-343_5min20/mtz004_PROC_1_XIA2_DIALS/di_w1_run1_anom_AUTOMATIC_DEFAULT_free.mtz / C2
cypD-438_1min/mtz001_PROC_1_autoPROC/ap_w1_run1_anom_truncate.mtz / P422
cypD-438_1min/mtz002_PROC_1_XIA2_DIALS/di_w1_run1_anom_AUTOMATIC_DEFAULT_free.mtz / C2221
cypD-440_5min/mtz001_PROC_1_autoPROC/ap_w1_run1_anom_truncate.mtz / P1
cypD-619_4min45/mtz001_PROC_1_EDNA_proc/ep_cypD-619_4min45_w1_run1_anom_truncate.mtz / P422
cypD-619_4min45/mtz002_PROC_1_XDSAPP/cypD-619_4min45_w1_1_F.mtz / P422
cypD-619_4min45/mtz003_PROC_1_XIA2_DIALS/di_w1_run1_anom_AUTOMATIC_DEFAULT_free.mtz / P4212
```

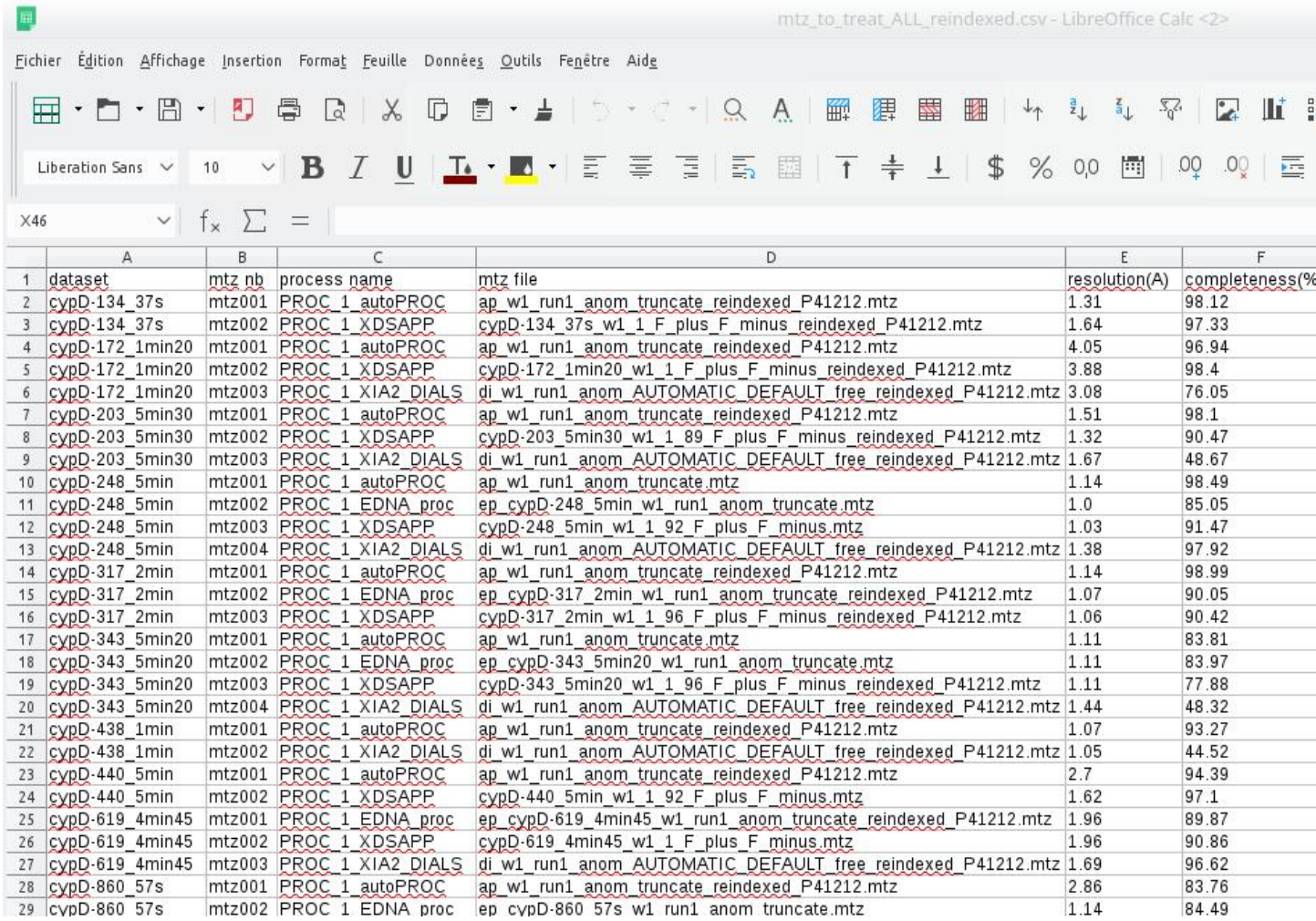
```
Number of reindexed mtz: 51
cypD-134_37s/mtz001_PROC_1_autoPROC/ap_w1_run1_anom_truncate_reindexed_P41212.mtz
cypD-203_5min30/mtz001_PROC_1_autoPROC/ap_w1_run1_anom_truncate_reindexed_P41212.mtz
cypD-203_5min30/mtz002_PROC_1_XDSAPP/cypD-203_5min30_w1_1_89_F_reindexed_P41212.mtz
cypD-248_5min/mtz003_PROC_1_XDSAPP/cypD-248_5min_w1_1_96_F_reindexed_P41212.mtz
cypD-317_2min/mtz001_PROC_1_autoPROC/ap_w1_run1_anom_truncate_reindexed_P41212.mtz
cypD-317_2min/mtz002_PROC_1_EDNA_proc/ep_cypD-317_2min_w1_run1_anom_truncate_reindexed_P41212.mtz
cypD-343_5min20/mtz003_PROC_1_XDSAPP/cypD-343_5min20_w1_1_96_F_reindexed_P41212.mtz
cypD-438_1min/mtz001_PROC_1_autoPROC/ap_w1_run1_anom_truncate_reindexed_P41212.mtz
cypD-619_4min45/mtz001_PROC_1_EDNA_proc/ep_cypD-619_4min45_w1_run1_anom_truncate_reindexed_P41212.mtz
cypD-619_4min45/mtz003_PROC_1_XIA2_DIALS/di_w1_run1_anom_AUTOMATIC_DEFAULT_free_reindexed_P41212.mtz
cypD-860_57s/mtz001_PROC_1_autoPROC/ap_w1_run1_anom_truncate_reindexed_P41212.mtz
cypD-863_2min30/mtz001_PROC_1_autoPROC/ap_w1_run1_anom_truncate_reindexed_P41212.mtz
cypD-864_1min/mtz001_PROC_1_autoPROC/ap_w1_run1_anom_truncate_reindexed_P41212.mtz
cypD-864_1min/mtz002_PROC_1_EDNA_proc/ep_cypD-864_1min_w1_run1_anom_truncate_reindexed_P41212.mtz
cypD-864_1min/mtz003_PROC_1_XDSAPP/cypD-864_1min_w1_1_95_F_reindexed_P41212.mtz
cypD-865_5min/mtz003_PROC_1_XDSAPP/cypD-865_5min_w1_1_96_F_reindexed_P41212.mtz
cypD-866_6min/mtz002_PROC_1_EDNA_proc/ep_cypD-866_6min_w1_run1_anom_truncate_reindexed_P41212.mtz
```

- launch xtriage[2] for each successfully reindexed mtz to get resolution, completeness, space group and cell parameters
- write a new 'mtz_to_treat_ALL_reindexed.csv' in '/easypipe/1b_reindex...' folder, with reindexed mtz files information

[2] https://www.phenix-online.org/documentation/reference/xtriage.html

	A	B	C	D	E	F	
1	dataset	mtz nb	process name	mtz file	resolution(A)	completeness(%)	spa
2	cypD-134_37s	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.31	97.98	P42
3	cypD-134_37s	mtz002	PROC_1_XDSAPP	cypD-134_37s_w1_1_F.mtz	1.64	42.53	P2
4	cypD-172_1min20	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	4.05	52.83	P1
5	cypD-172_1min20	mtz002	PROC_1_XDSAPP	cypD-172_1min20_w1_1_F.mtz	3.88	43.0	P1
6	cypD-172_1min20	mtz003	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free.mtz	3.08	71.63	P21
7	cypD-203_5min30	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.51	97.88	P42
8	cypD-203_5min30	mtz002	PROC_1_XDSAPP	cypD-203_5min30_w1_1_89_F.mtz	1.32	90.39	P42
9	cypD-203_5min30	mtz003	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free.mtz	1.67	83.63	C2
10	cypD-248_5min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.14	98.49	P41
11	cypD-248_5min	mtz002	PROC_1_EDNA_proc	ep_cypD-248_5min_w1_run1_anom_truncate.mtz	1.0	85.05	P41
12	cypD-248_5min	mtz003	PROC_1_XDSAPP	cypD-248_5min_w1_1_96_F.mtz	1.03	85.68	P43
13	cypD-248_5min	mtz004	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free.mtz	1.38	80.19	P2
14	cypD-317_2min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.14	98.9	P42
15	cypD-317_2min	mtz002	PROC_1_EDNA_proc	ep_cypD-317_2min_w1_run1_anom_truncate.mtz	1.07	95.13	P42
16	cypD-317_2min	mtz003	PROC_1_XDSAPP	cypD-317_2min_w1_1_92_F.mtz	1.06	90.43	P41
17	cypD-343_5min20	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.11	83.81	P41
18	cypD-343_5min20	mtz002	PROC_1_EDNA_proc	ep_cypD-343_5min20_w1_run1_anom_truncate.mtz	1.11	83.97	P41
19	cypD-343_5min20	mtz003	PROC_1_XDSAPP	cypD-343_5min20_w1_1_96_F.mtz	1.11	77.88	P43
20	cypD-343_5min20	mtz004	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free.mtz	1.44	83.17	C2
21	cypD-438_1min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.07	93.24	P42
22	cypD-438_1min	mtz002	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free.mtz	1.05	82.57	C22
23	cypD-440_5min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	2.7	57.25	P1
24	cypD-440_5min	mtz002	PROC_1_XDSAPP	cypD-440_5min_w1_1_92_F.mtz	1.62	96.57	P41
25	cypD-619_4min45	mtz001	PROC_1_EDNA_proc	ep_cypD-619_4min45_w1_run1_anom_truncate.mtz	1.96	90.86	P42
26	cypD-619_4min45	mtz002	PROC_1_XDSAPP	cypD-619_4min45_w1_1_F.mtz	1.96	90.86	P42
27	cypD-619_4min45	mtz003	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free.mtz	1.69	97.05	P42
28	cypD-860_57s	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	2.86	83.07	P42
29	cypD-860_57s	mtz002	PROC_1_EDNA_proc	ep_cypD-860_57s_w1_run1_anom_truncate.mtz	1.14	84.49	P41
30	cypD-860_57s	mtz003	PROC_1_XDSAPP	cypD-860_57s_w1_1_20_F.mtz	1.42	68.54	C22
31	cypD-860_57s	mtz004	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free.mtz	1.27	91.66	P22

becomes:



	A	B	C	D	E	F
1	dataset	mtz nb	process name	mtz file	resolution(A)	completeness(%
2	cypD-134_37s	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.31	98.12
3	cypD-134_37s	mtz002	PROC_1_XDSAPP	cypD-134_37s_w1_1_F_plus_F_minus_reindexed_P41212.mtz	1.64	97.33
4	cypD-172_1min20	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	4.05	96.94
5	cypD-172_1min20	mtz002	PROC_1_XDSAPP	cypD-172_1min20_w1_1_F_plus_F_minus_reindexed_P41212.mtz	3.88	98.4
6	cypD-172_1min20	mtz003	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free_reindexed_P41212.mtz	3.08	76.05
7	cypD-203_5min30	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.51	98.1
8	cypD-203_5min30	mtz002	PROC_1_XDSAPP	cypD-203_5min30_w1_1_89_F_plus_F_minus_reindexed_P41212.mtz	1.32	90.47
9	cypD-203_5min30	mtz003	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free_reindexed_P41212.mtz	1.67	48.67
10	cypD-248_5min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.14	98.49
11	cypD-248_5min	mtz002	PROC_1_EDNA_proc	ep_cypD-248_5min_w1_run1_anom_truncate.mtz	1.0	85.05
12	cypD-248_5min	mtz003	PROC_1_XDSAPP	cypD-248_5min_w1_1_92_F_plus_F_minus.mtz	1.03	91.47
13	cypD-248_5min	mtz004	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free_reindexed_P41212.mtz	1.38	97.92
14	cypD-317_2min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.14	98.99
15	cypD-317_2min	mtz002	PROC_1_EDNA_proc	ep_cypD-317_2min_w1_run1_anom_truncate_reindexed_P41212.mtz	1.07	90.05
16	cypD-317_2min	mtz003	PROC_1_XDSAPP	cypD-317_2min_w1_1_96_F_plus_F_minus_reindexed_P41212.mtz	1.06	90.42
17	cypD-343_5min20	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.11	83.81
18	cypD-343_5min20	mtz002	PROC_1_EDNA_proc	ep_cypD-343_5min20_w1_run1_anom_truncate.mtz	1.11	83.97
19	cypD-343_5min20	mtz003	PROC_1_XDSAPP	cypD-343_5min20_w1_1_96_F_plus_F_minus_reindexed_P41212.mtz	1.11	77.88
20	cypD-343_5min20	mtz004	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free_reindexed_P41212.mtz	1.44	48.32
21	cypD-438_1min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.07	93.27
22	cypD-438_1min	mtz002	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free_reindexed_P41212.mtz	1.05	44.52
23	cypD-440_5min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	2.7	94.39
24	cypD-440_5min	mtz002	PROC_1_XDSAPP	cypD-440_5min_w1_1_92_F_plus_F_minus.mtz	1.62	97.1
25	cypD-619_4min45	mtz001	PROC_1_EDNA_proc	ep_cypD-619_4min45_w1_run1_anom_truncate_reindexed_P41212.mtz	1.96	89.87
26	cypD-619_4min45	mtz002	PROC_1_XDSAPP	cypD-619_4min45_w1_1_F_plus_F_minus.mtz	1.96	90.86
27	cypD-619_4min45	mtz003	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free_reindexed_P41212.mtz	1.69	96.62
28	cypD-860_57s	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	2.86	83.76
29	cypD-860_57s	mtz002	PROC_1_EDNA_proc	ep_cypD-860_57s_w1_run1_anom_truncate.mtz	1.14	84.49

where P422, P4212 processed data have been successfully reindexed to P41212 space group.

Warning: If you run again 'prep' step for any reason like adding new datasets, you will have to run again this 'reindex' step. Even if they don't need to be reindexed, you have to run 'reindex' step to have the right reindexed csv file including these new datasets.

7.3 References

CHAPTER

EIGHT

EASYPIPE 'LIGANDS'

This step is mandatory if you want Phenix to search ligand, else it is optional.

'ligands' subcommand generates pdb and cif from smiles with eLBOW[2] .

Important: First, template csv file generated with 'prep' subcommand' have to be completed with ligands names and smiles.

8.1 Usage

easypipe.py data ligands [-h] ligands_csv

arguments	description
-h, –help	show this help message and exit
ligands_csv	ligands_for_datasets.csv file from 'prep' with ligands names and smiles completed (mandatory)

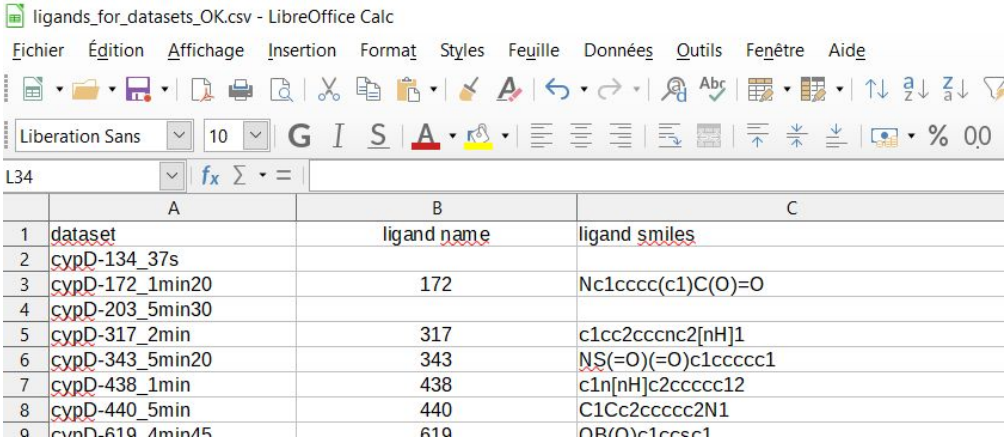
Example:

```
$ easypipe.py PROCESSED_DATA ligands easYPipe/1c_ligands/ligands_for_datasets_OK.csv
```

8.2 What does it do ?

- First, you have to fill in the fields 'ligand name' and 'ligand smiles' of /1c_ligands/ligands_for_datasets.csv csv file, then save the csv file somewhere else or with another name if you don't want to overwrite it in case you run 'prep' subcommand again . . .

[2] https://www.phenix-online.org/documentation/reference/elbow.html


ligands_for_datasets_OK.csv - LibreOffice Calc

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Liberation Sans 10

L34

	A	B	C
1	dataset	ligand name	ligand smiles
2	cypD-134_37s		
3	cypD-172_1min20	172	Nc1cccc(c1)C(O)=O
4	cypD-203_5min30		
5	cypD-317_2min	317	c1cc2cccnc2[nH]1
6	cypD-343_5min20	343	NS(=O)(=O)c1ccccc1
7	cypD-438_1min	438	c1n[nH]c2ccccc12
8	cypD-440_5min	440	C1Cc2ccccc2N1
9	cypD-619_4min45	619	OB(O)c1ccsc1

- 'ligands' subcommand generates pdb and cif of ligands and copies them in corresponding processed dataset folders, in a 'ligand' folder. It first creates a smiles file accordingly to the ligands_csv input, canonizes it thanks to Open Babel[1] and converts it with eLBOW[2] to pdb and cif.

[1] http://openbabel.org/wiki/Main_Page

```
0_processed_datasets/
├── cypD-134_37s
│   ├── data
│   │   ├── mtz001_PROC_1_autoPROC
│   │   │   ├── ap_w1_run1_anom_truncate.mtz
│   │   │   ├── ap_w1_run1_anom_truncate.mtz.old
│   │   │   ├── ap_w1_run1_anom_truncate_reindexed_P41212.mtz
│   │   │   ├── xtriage_ap_w1_run1_anom_truncate.log
│   │   │   ├── xtriage-verbose_labels.log
│   │   │   └── xtriage-verbose.log
│   │   └── mtz002_PROC_1_XDSAPP
│   │       ├── cypD-134_37s_w1_1_F_plus_F_minus.mtz
│   │       ├── xtriage_cypD-134_37s_w1_1_F_plus_F_minus.log
│   │       ├── xtriage-verbose_labels.log
│   │       └── xtriage-verbose.log
│   └── ligand
├── cypD-172_1min20
│   ├── data
│   │   ├── mtz001_PROC_1_autoPROC
│   │   │   ├── ap_w1_run1_anom_truncate.mtz
│   │   │   ├── xtriage_ap_w1_run1_anom_truncate.log
│   │   │   ├── xtriage-verbose_labels.log
│   │   │   └── xtriage-verbose.log
│   │   ├── mtz002_PROC_1_XDSAPP
│   │   │   ├── cypD-172_1min20_w1_1_F_plus_F_minus.mtz
│   │   │   ├── xtriage_cypD-172_1min20_w1_1_F_plus_F_minus.log
│   │   │   ├── xtriage-verbose_labels.log
│   │   │   └── xtriage-verbose.log
│   │   └── mtz003_PROC_1_XIA2_DIALS
│   │       ├── di_w1_run1_anom_AUTOMATIC_DEFAULT_free.mtz
│   │       ├── xtriage_di_w1_run1_anom_AUTOMATIC_DEFAULT_free.log
│   │       ├── xtriage-verbose_labels.log
│   │       └── xtriage-verbose.log
│   └── ligand
│       ├── 172.cif
│       ├── 172.elbow_opt.xyz
│       ├── 172.options.pickle
│       ├── 172.pdb
│       ├── 172.pickle
│       └── 172.smi
├── cypD-203_5min30
```

Important: If eLBOW[2] fails to generate pdb and cif from smiles, you can copy your own cif in ligand sub-folder of the corresponding dataset, eLBOW[2] will generate pdb from this cif.

8.3 References

CHAPTER

NINE

EASYPIPE 'LAUNCH'

'launch' subcommand runs phenix.ligand_pipeline[1] on all the mtz (several processed data, several datasets) according to options and information in 'mtz_to_treat_ALL.csv' file.

9.1 Usage

easypipe.py data launch [-h] [-m {fast,full,allsg}] [-l] [-n NUMBER] [-c NUMBER] [-b NUMBER | -a] [-s] [-t TEMPLATE] ref

arguments	description
ref	folder with fasta file and pdb file for replacement, and cif(s) if ligand(s) in the model

Warning: reference pdb files should include the row starting with 'CRYST1' containing information on space group

optional arguments	description
-h, –help	show this help message and exit
-m {fast,full,allsg}, –mode {fast,full,allsg}	running mode: fast, full, or allsg (default = fast)
-l, –lig	for ligand search and placement
-n NUMBER, –nblig NUMBER	number of ligand copies to be searched (default = 1, max 9 for the moment).
-c NUMBER, –cclig NUMBER	minimum CC to consider a ligand placement correct (default = 0.7). Ligands with at least this CC will be incorporated into the current model for refinement.
-b NUMBER, –best NUMBER	launch only for mtz with best completeness, NUMBER indicates how many mtz to treat (default 1), ex: –best 2
-a, –autoproc	launch only for mtz from autoPROC, or if none launch for mtz with best completeness
-w, –whole	launch for the whole mtz processes
-s, –simulate	only simulate, generate a csv file according to the future launch options. Give the possibility to modify the csv file to choose not to launch certain treatments, before restarting without simulation mode.
-t TEMPLATE, –template TEMPLATE	optional template name for log files and result folders, in case re-launching with different reference pdb of the same space group (else will overwrite).

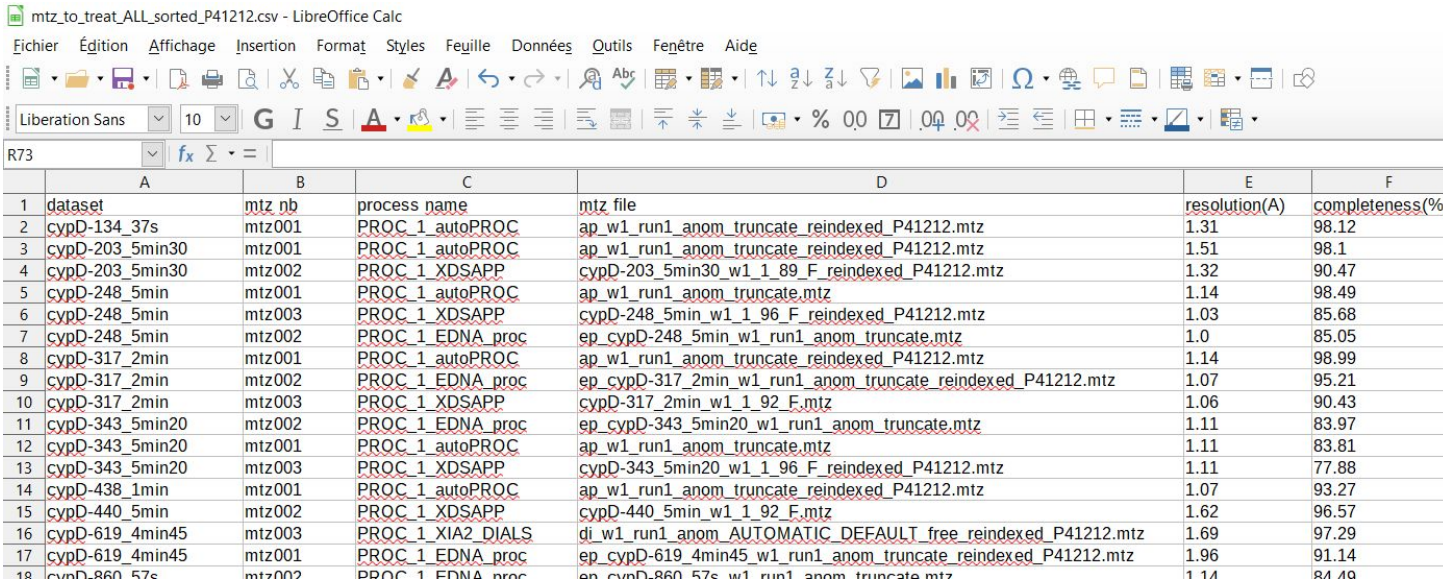
[1] https://www.phenix-online.org/documentation/reference/ligand_pipeline.html

Example:

```
$ easypipe.py PROCESSED_DATA launch my_ref_folder --mode full --lig --best 2 --cclig␣
↪0.6
equivalent to:
$ easypipe.py PROCESSED_DATA launch my_ref_folder -m full -l -b 2 -c 0.6
```

9.2 What does it do ?

9.2.1 1. Sort mtz files according to space group in reference pdb, and decreasing completeness



mtz_to_treat_ALL_sorted_P41212.csv - LibreOffice Calc

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Liberation Sans 10

R73

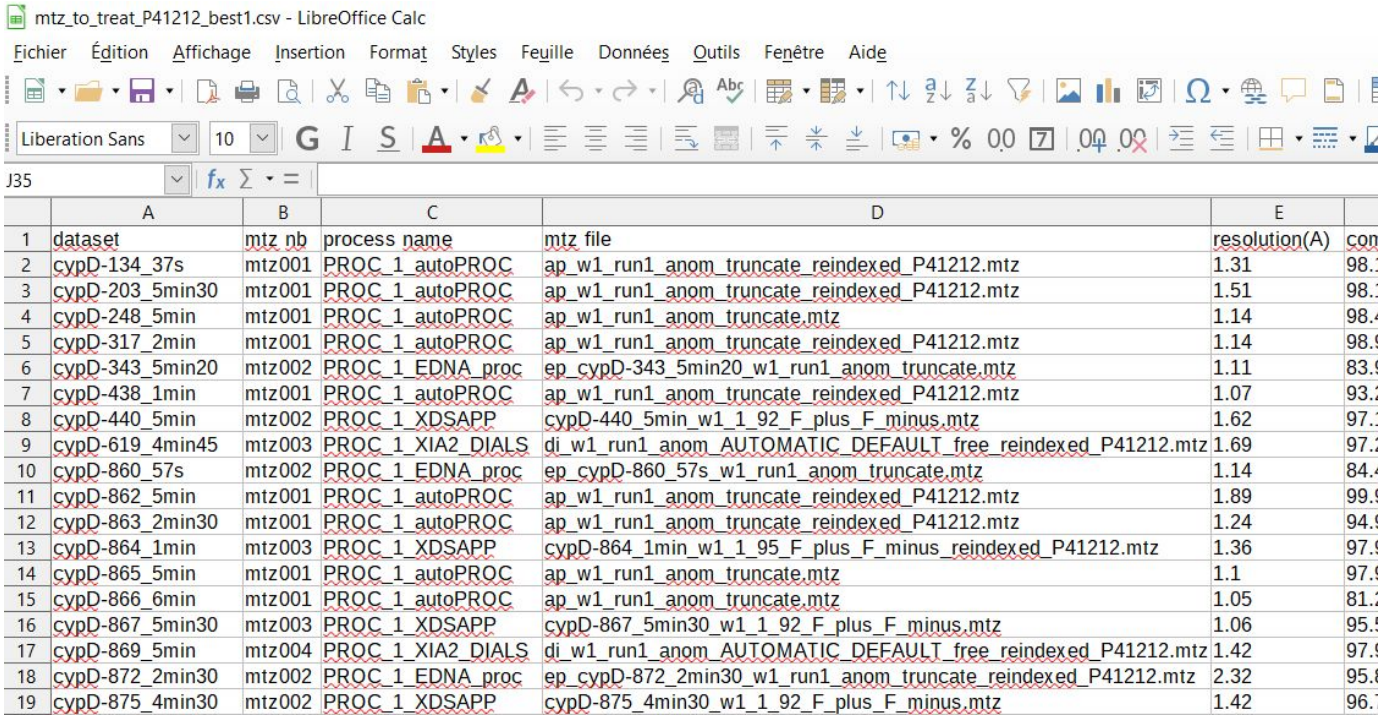
	A	B	C	D	E	F
1	dataset	mtz nb	process name	mtz file	resolution(A)	completeness(%
2	cypD-134_37s	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.31	98.12
3	cypD-203_5min30	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.51	98.1
4	cypD-203_5min30	mtz002	PROC_1_XDSAPP	cypD-203_5min30_w1_1_89_F_reindexed_P41212.mtz	1.32	90.47
5	cypD-248_5min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.14	98.49
6	cypD-248_5min	mtz003	PROC_1_XDSAPP	cypD-248_5min_w1_1_96_F_reindexed_P41212.mtz	1.03	85.68
7	cypD-248_5min	mtz002	PROC_1_EDNA_proc	ep_cypD-248_5min_w1_run1_anom_truncate.mtz	1.0	85.05
8	cypD-317_2min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.14	98.99
9	cypD-317_2min	mtz002	PROC_1_EDNA_proc	ep_cypD-317_2min_w1_run1_anom_truncate_reindexed_P41212.mtz	1.07	95.21
10	cypD-317_2min	mtz003	PROC_1_XDSAPP	cypD-317_2min_w1_1_92_F.mtz	1.06	90.43
11	cypD-343_5min20	mtz002	PROC_1_EDNA_proc	ep_cypD-343_5min20_w1_run1_anom_truncate.mtz	1.11	83.97
12	cypD-343_5min20	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.11	83.81
13	cypD-343_5min20	mtz003	PROC_1_XDSAPP	cypD-343_5min20_w1_1_96_F_reindexed_P41212.mtz	1.11	77.88
14	cypD-438_1min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.07	93.27
15	cypD-440_5min	mtz002	PROC_1_XDSAPP	cypD-440_5min_w1_1_92_F.mtz	1.62	96.57
16	cypD-619_4min45	mtz003	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free_reindexed_P41212.mtz	1.69	97.29
17	cypD-619_4min45	mtz001	PROC_1_EDNA_proc	ep_cypD-619_4min45_w1_run1_anom_truncate_reindexed_P41212.mtz	1.96	91.14
18	cypD-860_57s	mtz002	PROC_1_EDNA_proc	ep_cypD-860_57s_w1_run1_anom_truncate.mtz	1.14	84.49

If there are datasets without any mtz to treat according to space group, these datasets are listed in another csv file ("datasets_without_mtz_<sg_ref>.csv").

9.2.2 2. List mtz files according to option 'best', 'autoproc' or 'whole'

- Option example: –best 1 (default)

List only mtz with best completeness for each dataset.


mtz_to_treat_P41212_best1.csv - LibreOffice Calc

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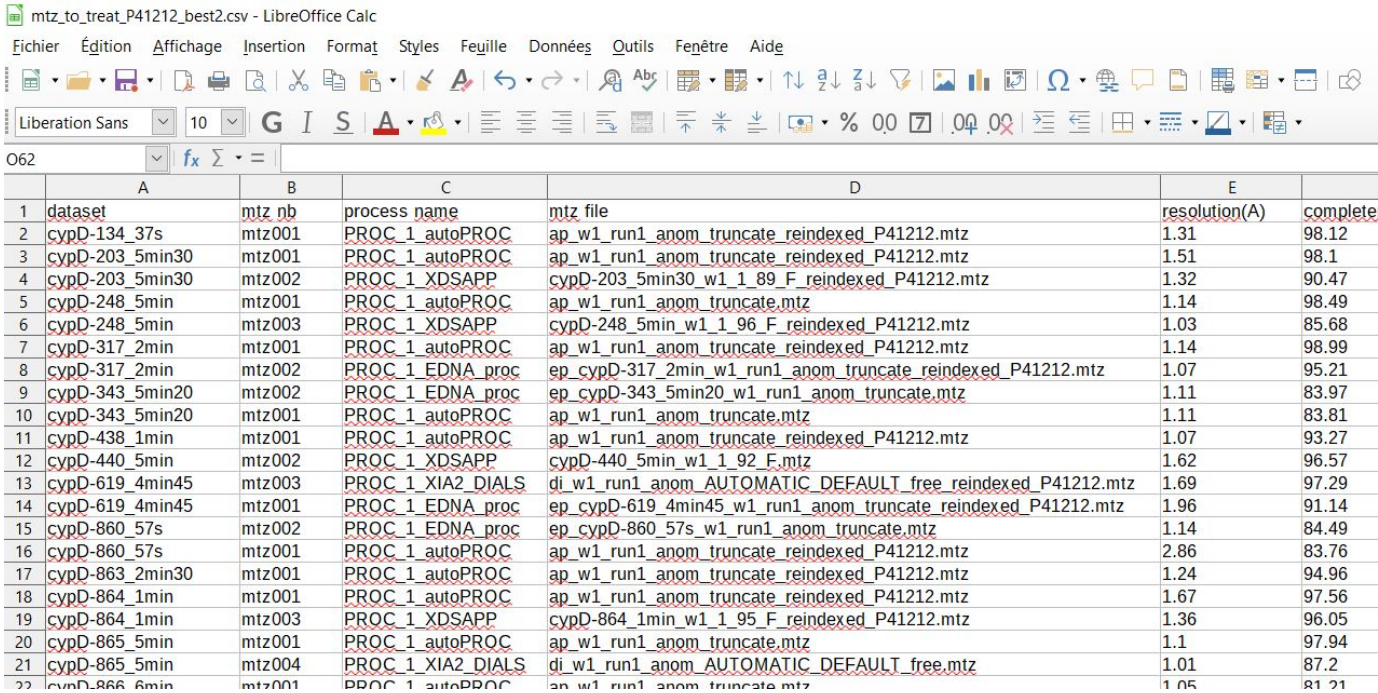
Liberation Sans 10

J35

	A	B	C	D	E
1	dataset	mtz nb	process name	mtz file	resolution(A)
2	cypD-134_37s	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.31
3	cypD-203_5min30	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.51
4	cypD-248_5min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.14
5	cypD-317_2min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.14
6	cypD-343_5min20	mtz002	PROC_1_EDNA_proc	ep_cypD-343_5min20_w1_run1_anom_truncate.mtz	1.11
7	cypD-438_1min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.07
8	cypD-440_5min	mtz002	PROC_1_XDSAPP	cypD-440_5min_w1_1_92_F_plus_F_minus.mtz	1.62
9	cypD-619_4min45	mtz003	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free_reindexed_P41212.mtz	1.69
10	cypD-860_57s	mtz002	PROC_1_EDNA_proc	ep_cypD-860_57s_w1_run1_anom_truncate.mtz	1.14
11	cypD-862_5min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.89
12	cypD-863_2min30	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.24
13	cypD-864_1min	mtz003	PROC_1_XDSAPP	cypD-864_1min_w1_1_95_F_plus_F_minus_reindexed_P41212.mtz	1.36
14	cypD-865_5min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.1
15	cypD-866_6min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.05
16	cypD-867_5min30	mtz003	PROC_1_XDSAPP	cypD-867_5min30_w1_1_92_F_plus_F_minus.mtz	1.06
17	cypD-869_5min	mtz004	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free_reindexed_P41212.mtz	1.42
18	cypD-872_2min30	mtz002	PROC_1_EDNA_proc	ep_cypD-872_2min30_w1_run1_anom_truncate_reindexed_P41212.mtz	2.32
19	cypD-875_4min30	mtz002	PROC_1_XDSAPP	cypD-875_4min30_w1_1_92_F_plus_F_minus.mtz	1.42

- Option example: –best 2

List only 2 first mtz, when exist, with best completeness, for each dataset.


mtz_to_treat_P41212_best2.csv - LibreOffice Calc

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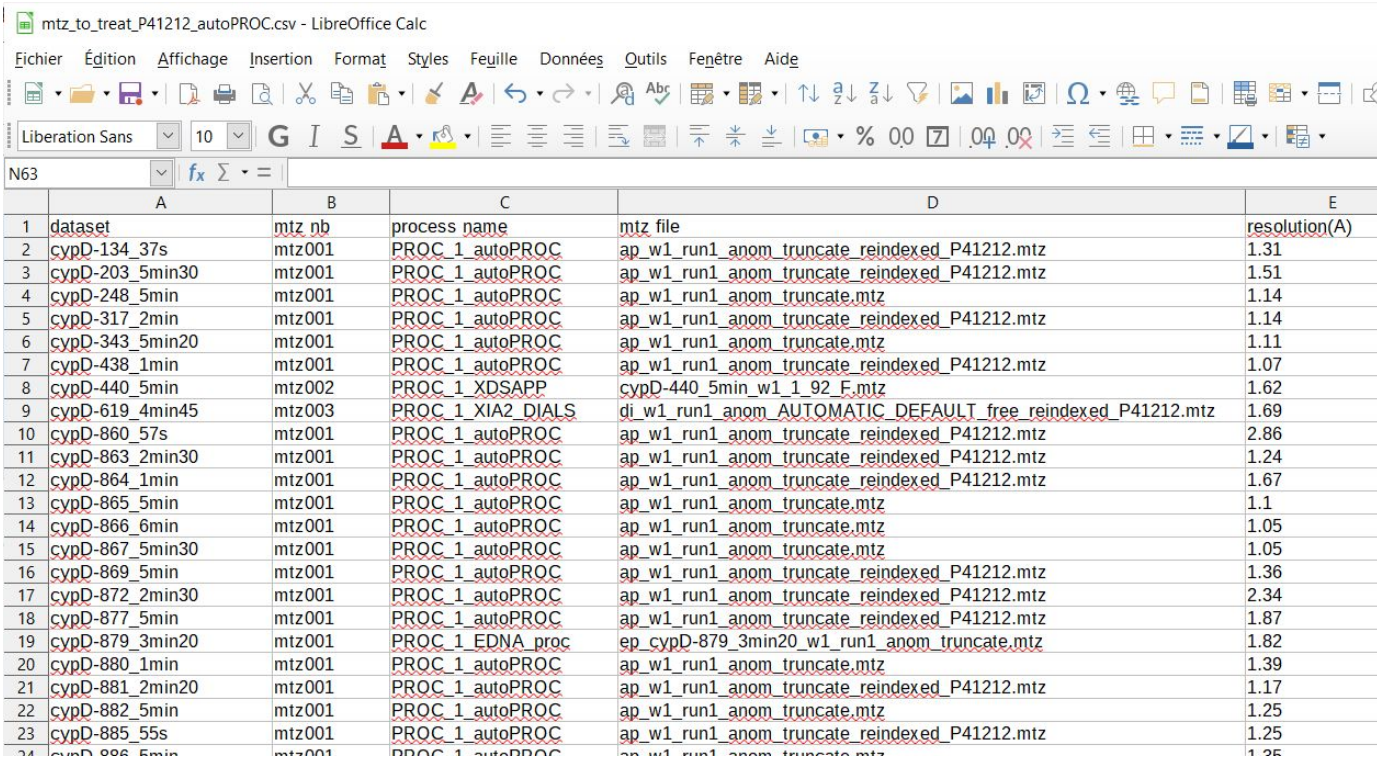
Liberation Sans 10

O62

	A	B	C	D	E
1	dataset	mtz nb	process name	mtz file	resolution(A)
2	cypD-134_37s	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.31
3	cypD-203_5min30	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.51
4	cypD-203_5min30	mtz002	PROC_1_XDSAPP	cypD-203_5min30_w1_1_89_F_reindexed_P41212.mtz	1.32
5	cypD-248_5min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.14
6	cypD-248_5min	mtz003	PROC_1_XDSAPP	cypD-248_5min_w1_1_96_F_reindexed_P41212.mtz	1.03
7	cypD-317_2min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.14
8	cypD-317_2min	mtz002	PROC_1_EDNA_proc	ep_cypD-317_2min_w1_run1_anom_truncate_reindexed_P41212.mtz	1.07
9	cypD-343_5min20	mtz002	PROC_1_EDNA_proc	ep_cypD-343_5min20_w1_run1_anom_truncate.mtz	1.11
10	cypD-343_5min20	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.11
11	cypD-438_1min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.07
12	cypD-440_5min	mtz002	PROC_1_XDSAPP	cypD-440_5min_w1_1_92_F.mtz	1.62
13	cypD-619_4min45	mtz003	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free_reindexed_P41212.mtz	1.69
14	cypD-619_4min45	mtz001	PROC_1_EDNA_proc	ep_cypD-619_4min45_w1_run1_anom_truncate_reindexed_P41212.mtz	1.96
15	cypD-860_57s	mtz002	PROC_1_EDNA_proc	ep_cypD-860_57s_w1_run1_anom_truncate.mtz	1.14
16	cypD-860_57s	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	2.86
17	cypD-863_2min30	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.24
18	cypD-864_1min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.67
19	cypD-864_1min	mtz003	PROC_1_XDSAPP	cypD-864_1min_w1_1_95_F_reindexed_P41212.mtz	1.36
20	cypD-865_5min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.1
21	cypD-865_5min	mtz004	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free.mtz	1.01

- Option example: –autoproc

List only mtz from autoPROC, or if none list mtz with best completeness, for each dataset.


mtz_to_treat_P41212_autoPROC.csv - LibreOffice Calc

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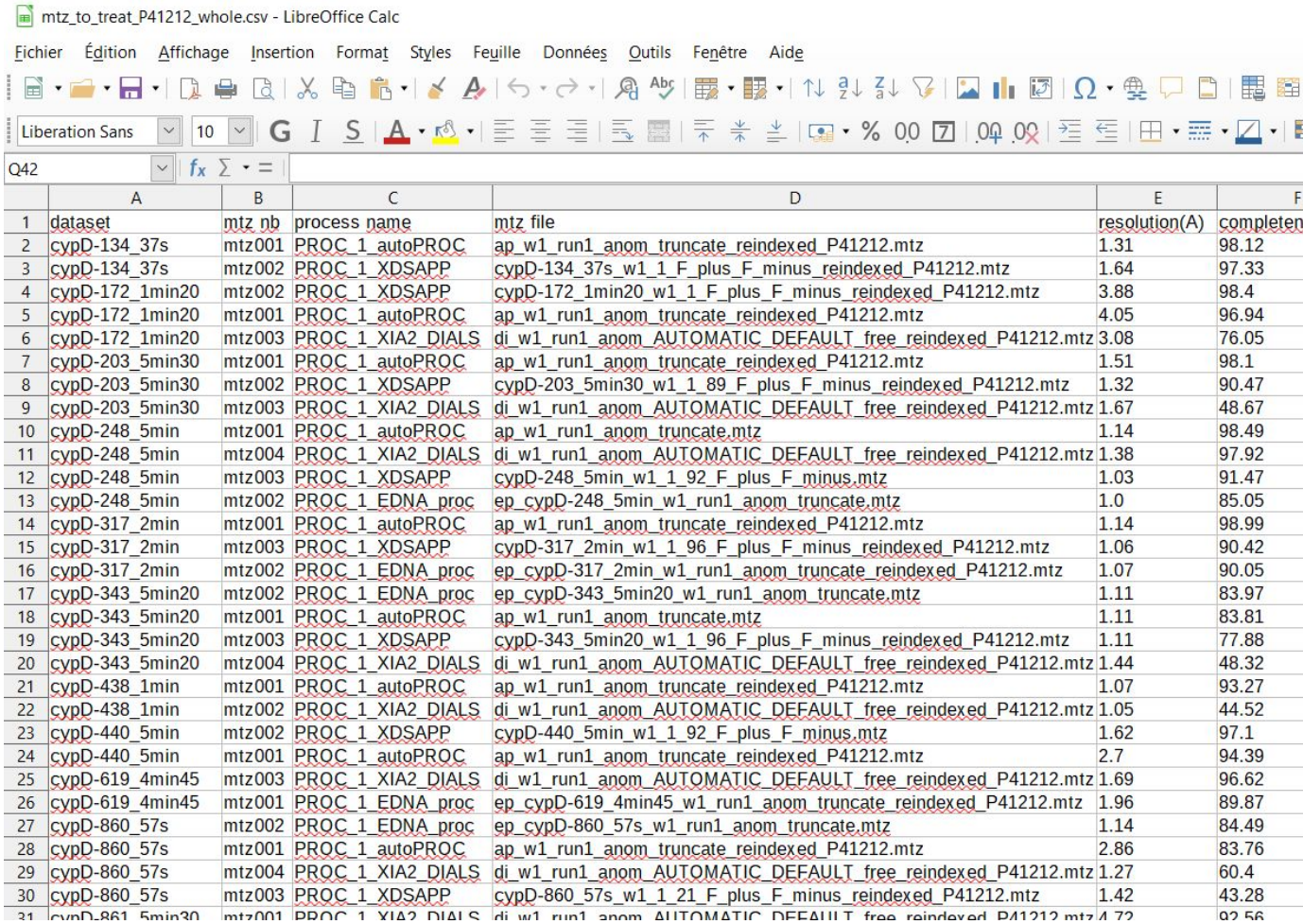
Liberation Sans 10

N63

	A	B	C	D	E
1	dataset	mtz nb	process name	mtz file	resolution(A)
2	cypD-134_37s	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.31
3	cypD-203_5min30	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.51
4	cypD-248_5min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.14
5	cypD-317_2min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.14
6	cypD-343_5min20	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.11
7	cypD-438_1min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.07
8	cypD-440_5min	mtz002	PROC_1_XDSAPP	cypD-440_5min_w1_1_92_F.mtz	1.62
9	cypD-619_4min45	mtz003	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free_reindexed_P41212.mtz	1.69
10	cypD-860_57s	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	2.86
11	cypD-863_2min30	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.24
12	cypD-864_1min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.67
13	cypD-865_5min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.1
14	cypD-866_6min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.05
15	cypD-867_5min30	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.05
16	cypD-869_5min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.36
17	cypD-872_2min30	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	2.34
18	cypD-877_5min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.87
19	cypD-879_3min20	mtz001	PROC_1_EDNA_proc	ep_cypD-879_3min20_w1_run1_anom_truncate.mtz	1.82
20	cypD-880_1min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.39
21	cypD-881_2min20	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.17
22	cypD-882_5min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.25
23	cypD-885_55s	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.25

- Option example: –whole

Whereas it is not recommended because it is time demanding, for problematic data it could be usefull to treat the whole mtz processed.



mtz_to_treat_P41212_whole.csv - LibreOffice Calc

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Liberation Sans 10

Q42

	A	B	C	D	E	F
1	dataset	mtz nb	process name	mtz file	resolution(A)	completen
2	cypD-134_37s	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.31	98.12
3	cypD-134_37s	mtz002	PROC_1_XDSAPP	cypD-134_37s_w1_1_F_plus_F_minus_reindexed_P41212.mtz	1.64	97.33
4	cypD-172_1min20	mtz002	PROC_1_XDSAPP	cypD-172_1min20_w1_1_F_plus_F_minus_reindexed_P41212.mtz	3.88	98.4
5	cypD-172_1min20	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	4.05	96.94
6	cypD-172_1min20	mtz003	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free_reindexed_P41212.mtz	3.08	76.05
7	cypD-203_5min30	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.51	98.1
8	cypD-203_5min30	mtz002	PROC_1_XDSAPP	cypD-203_5min30_w1_1_89_F_plus_F_minus_reindexed_P41212.mtz	1.32	90.47
9	cypD-203_5min30	mtz003	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free_reindexed_P41212.mtz	1.67	48.67
10	cypD-248_5min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.14	98.49
11	cypD-248_5min	mtz004	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free_reindexed_P41212.mtz	1.38	97.92
12	cypD-248_5min	mtz003	PROC_1_XDSAPP	cypD-248_5min_w1_1_92_F_plus_F_minus.mtz	1.03	91.47
13	cypD-248_5min	mtz002	PROC_1_EDNA_proc	ep_cypD-248_5min_w1_run1_anom_truncate.mtz	1.0	85.05
14	cypD-317_2min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.14	98.99
15	cypD-317_2min	mtz003	PROC_1_XDSAPP	cypD-317_2min_w1_1_96_F_plus_F_minus_reindexed_P41212.mtz	1.06	90.42
16	cypD-317_2min	mtz002	PROC_1_EDNA_proc	ep_cypD-317_2min_w1_run1_anom_truncate_reindexed_P41212.mtz	1.07	90.05
17	cypD-343_5min20	mtz002	PROC_1_EDNA_proc	ep_cypD-343_5min20_w1_run1_anom_truncate.mtz	1.11	83.97
18	cypD-343_5min20	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate.mtz	1.11	83.81
19	cypD-343_5min20	mtz003	PROC_1_XDSAPP	cypD-343_5min20_w1_1_96_F_plus_F_minus_reindexed_P41212.mtz	1.11	77.88
20	cypD-343_5min20	mtz004	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free_reindexed_P41212.mtz	1.44	48.32
21	cypD-438_1min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	1.07	93.27
22	cypD-438_1min	mtz002	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free_reindexed_P41212.mtz	1.05	44.52
23	cypD-440_5min	mtz002	PROC_1_XDSAPP	cypD-440_5min_w1_1_92_F_plus_F_minus.mtz	1.62	97.1
24	cypD-440_5min	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	2.7	94.39
25	cypD-619_4min45	mtz003	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free_reindexed_P41212.mtz	1.69	96.62
26	cypD-619_4min45	mtz001	PROC_1_EDNA_proc	ep_cypD-619_4min45_w1_run1_anom_truncate_reindexed_P41212.mtz	1.96	89.87
27	cypD-860_57s	mtz002	PROC_1_EDNA_proc	ep_cypD-860_57s_w1_run1_anom_truncate.mtz	1.14	84.49
28	cypD-860_57s	mtz001	PROC_1_autoPROC	ap_w1_run1_anom_truncate_reindexed_P41212.mtz	2.86	83.76
29	cypD-860_57s	mtz004	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free_reindexed_P41212.mtz	1.27	60.4
30	cypD-860_57s	mtz003	PROC_1_XDSAPP	cypD-860_57s_w1_1_21_F_plus_F_minus_reindexed_P41212.mtz	1.42	43.28
31	cypD-861_5min30	mtz001	PROC_1_XIA2_DIALS	di_w1_run1_anom_AUTOMATIC_DEFAULT_free_reindexed_P41212.mtz	4.72	92.56

9.2.3 3. List mtz files with mode and ligand information for running Phenix

Note: Phenix options for the different modes are specified *hereafter*.

For each dataset, write in a 'launch csv' file:

- if ligand cif file is present for search when asked
- mode that will be launched depending on mode asked, the presence (or not) of ligand cif file and data quality
- information in case mode is different from mode asked
- result folder name

Limits for poor data: There are minimum limits to process in 'full' or 'allsg' modes. These limits can be modified in config.py file (after what easypipe should be reinstalled).

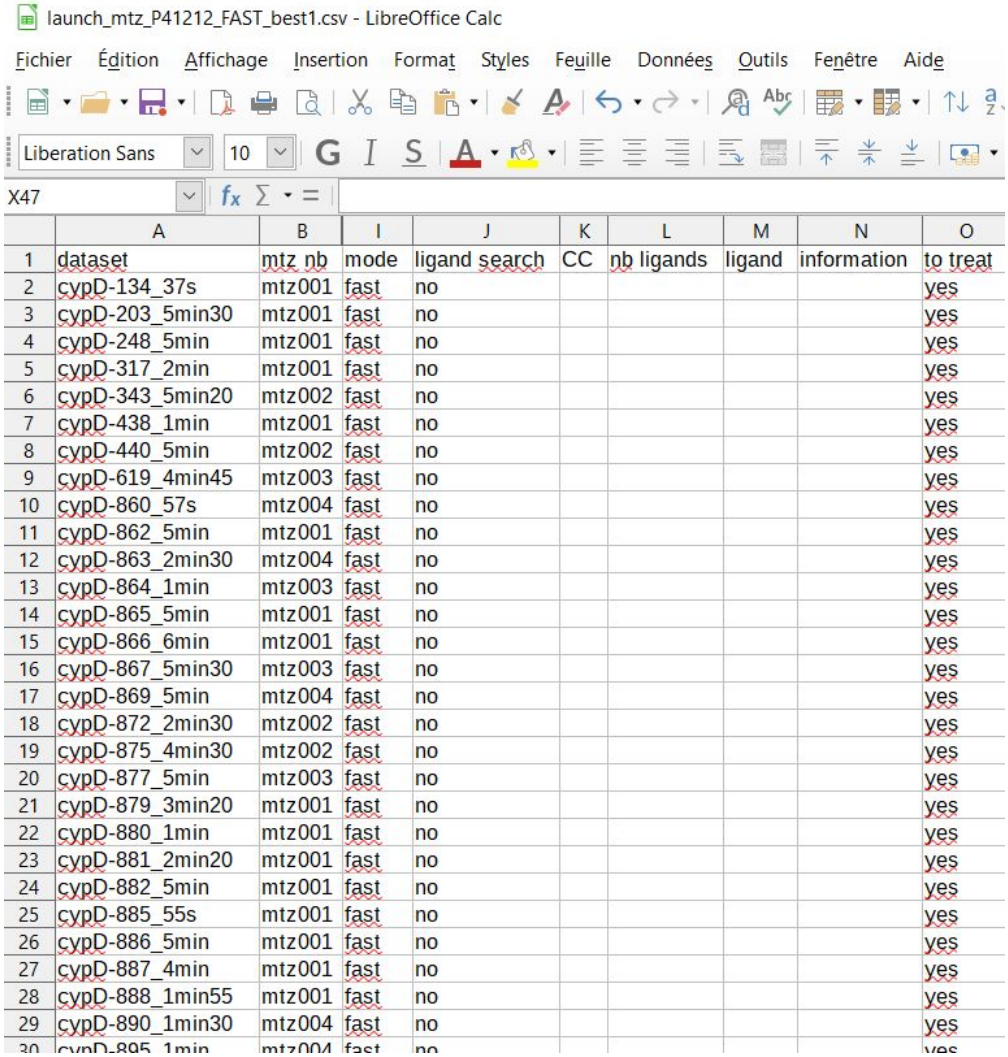
- minimum completeness (default = 70%)
- minimum resolution (default = 3.75)

Poor data will be treated in 'fast' mode.

Option examples:

- Option example: –mode fast (default)

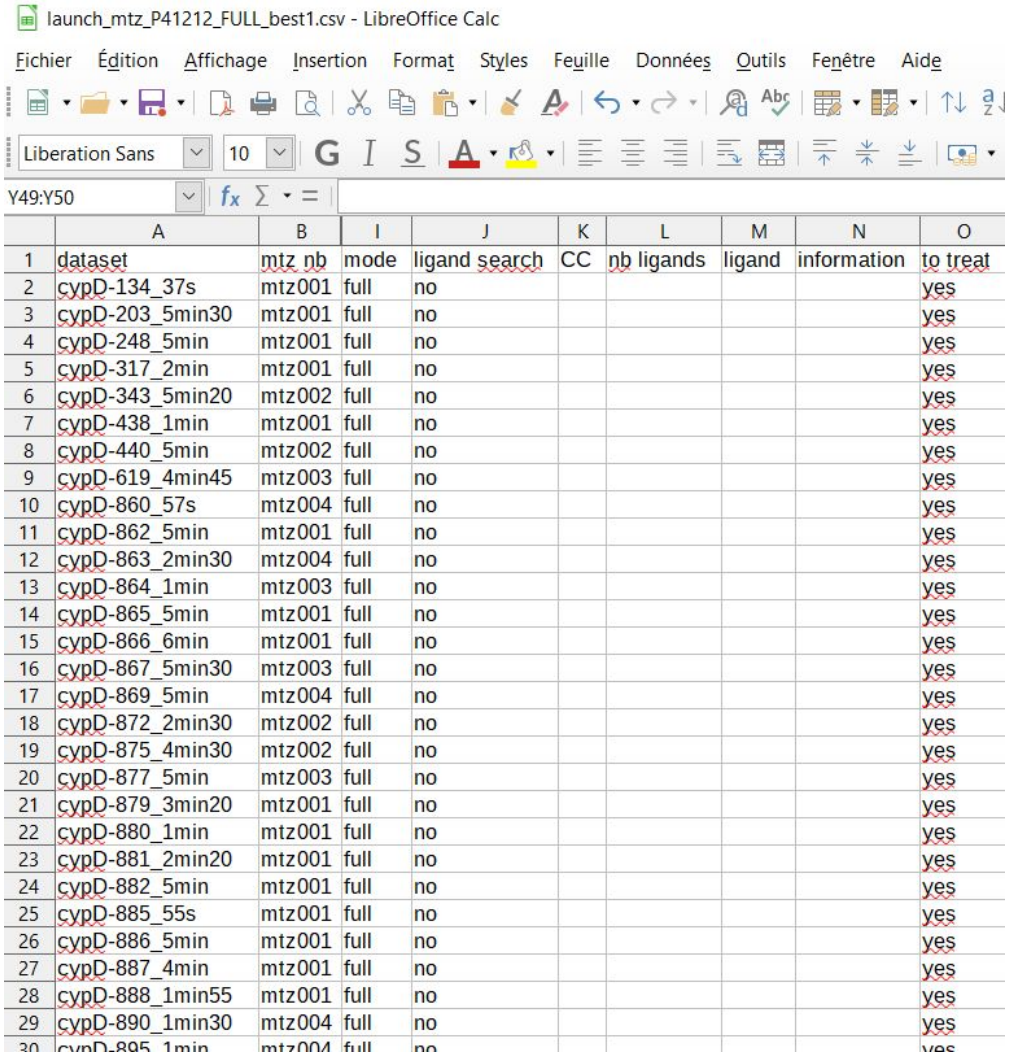
Phenix uses a simple rigid-body refinement for model placement, which is faster and most of the time sufficient if the input model is already close enough to the target structure.



	A	B	I	J	K	L	M	N	O
1	dataset	mtz nb	mode	ligand search	CC	nb ligands	ligand	information	to treat
2	cypD-134_37s	mtz001	fast	no					yes
3	cypD-203_5min30	mtz001	fast	no					yes
4	cypD-248_5min	mtz001	fast	no					yes
5	cypD-317_2min	mtz001	fast	no					yes
6	cypD-343_5min20	mtz002	fast	no					yes
7	cypD-438_1min	mtz001	fast	no					yes
8	cypD-440_5min	mtz002	fast	no					yes
9	cypD-619_4min45	mtz003	fast	no					yes
10	cypD-860_57s	mtz004	fast	no					yes
11	cypD-862_5min	mtz001	fast	no					yes
12	cypD-863_2min30	mtz004	fast	no					yes
13	cypD-864_1min	mtz003	fast	no					yes
14	cypD-865_5min	mtz001	fast	no					yes
15	cypD-866_6min	mtz001	fast	no					yes
16	cypD-867_5min30	mtz003	fast	no					yes
17	cypD-869_5min	mtz004	fast	no					yes
18	cypD-872_2min30	mtz002	fast	no					yes
19	cypD-875_4min30	mtz002	fast	no					yes
20	cypD-877_5min	mtz003	fast	no					yes
21	cypD-879_3min20	mtz001	fast	no					yes
22	cypD-880_1min	mtz001	fast	no					yes
23	cypD-881_2min20	mtz001	fast	no					yes
24	cypD-882_5min	mtz001	fast	no					yes
25	cypD-885_55s	mtz001	fast	no					yes
26	cypD-886_5min	mtz001	fast	no					yes
27	cypD-887_4min	mtz001	fast	no					yes
28	cypD-888_1min55	mtz001	fast	no					yes
29	cypD-890_1min30	mtz004	fast	no					yes
30	cypD-895_1min	mtz004	fast	no					yes

- Option example: –mode full

Phenix will try rigid-body refinement first, then run Phaser if the R-free is too high (>0.4), it will run AutoBuild after initial refinement only if R-free is greater than the max_r_free cutoff = 0.3.



launch_mtz_P41212_FULL_best1.csv - LibreOffice Calc

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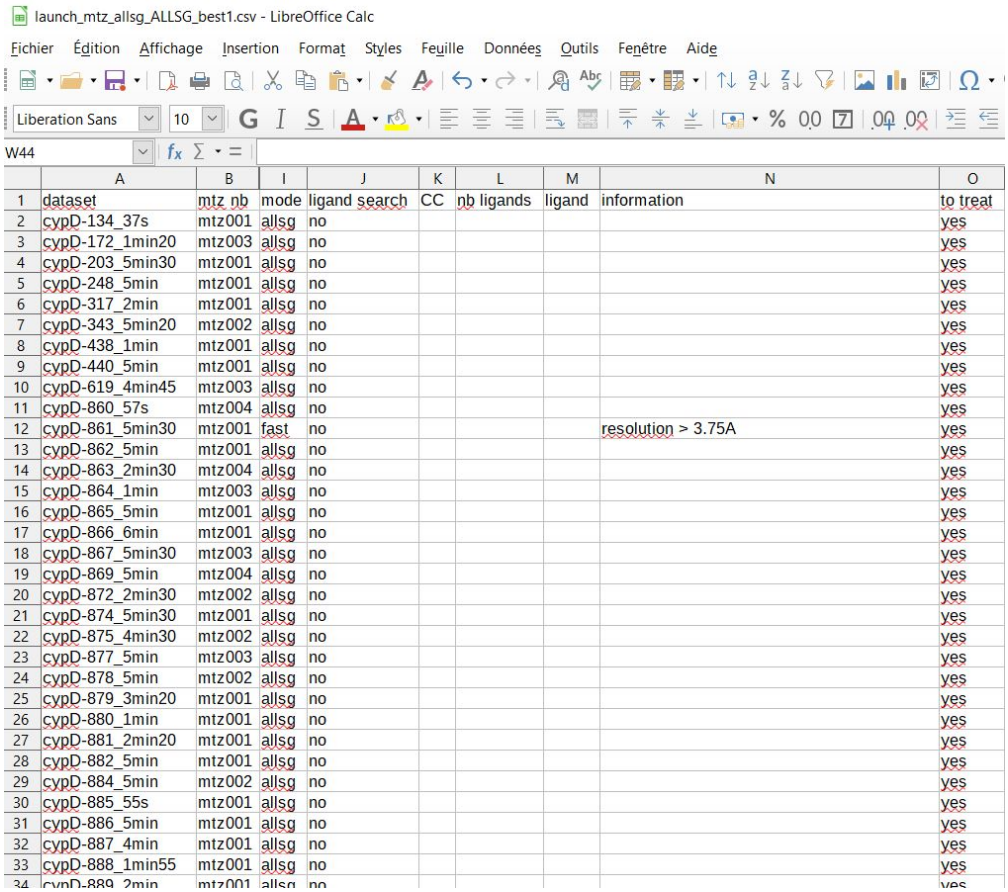
Liberation Sans 10

Y49:Y50

	A	B	I	J	K	L	M	N	O
1	dataset	mtz nb	mode	ligand search	CC	nb ligands	ligand	information	to treat
2	cypD-134_37s	mtz001	full	no					yes
3	cypD-203_5min30	mtz001	full	no					yes
4	cypD-248_5min	mtz001	full	no					yes
5	cypD-317_2min	mtz001	full	no					yes
6	cypD-343_5min20	mtz002	full	no					yes
7	cypD-438_1min	mtz001	full	no					yes
8	cypD-440_5min	mtz002	full	no					yes
9	cypD-619_4min45	mtz003	full	no					yes
10	cypD-860_57s	mtz004	full	no					yes
11	cypD-862_5min	mtz001	full	no					yes
12	cypD-863_2min30	mtz004	full	no					yes
13	cypD-864_1min	mtz003	full	no					yes
14	cypD-865_5min	mtz001	full	no					yes
15	cypD-866_6min	mtz001	full	no					yes
16	cypD-867_5min30	mtz003	full	no					yes
17	cypD-869_5min	mtz004	full	no					yes
18	cypD-872_2min30	mtz002	full	no					yes
19	cypD-875_4min30	mtz002	full	no					yes
20	cypD-877_5min	mtz003	full	no					yes
21	cypD-879_3min20	mtz001	full	no					yes
22	cypD-880_1min	mtz001	full	no					yes
23	cypD-881_2min20	mtz001	full	no					yes
24	cypD-882_5min	mtz001	full	no					yes
25	cypD-885_55s	mtz001	full	no					yes
26	cypD-886_5min	mtz001	full	no					yes
27	cypD-887_4min	mtz001	full	no					yes
28	cypD-888_1min55	mtz001	full	no					yes
29	cypD-890_1min30	mtz004	full	no					yes
30	cypD-895_1min	mtz004	full	no					yes

- Option example: –mode allsg

In this mode, mtz will be treated regardless of the space group. Phenix will run Phaser, then run AutoBuild after initial refinement only if R-free is greater than the max_r_free cutoff = 0.3.


launch_mtz_allsg_ALLSG_best1.csv - LibreOffice Calc

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Liberation Sans 10

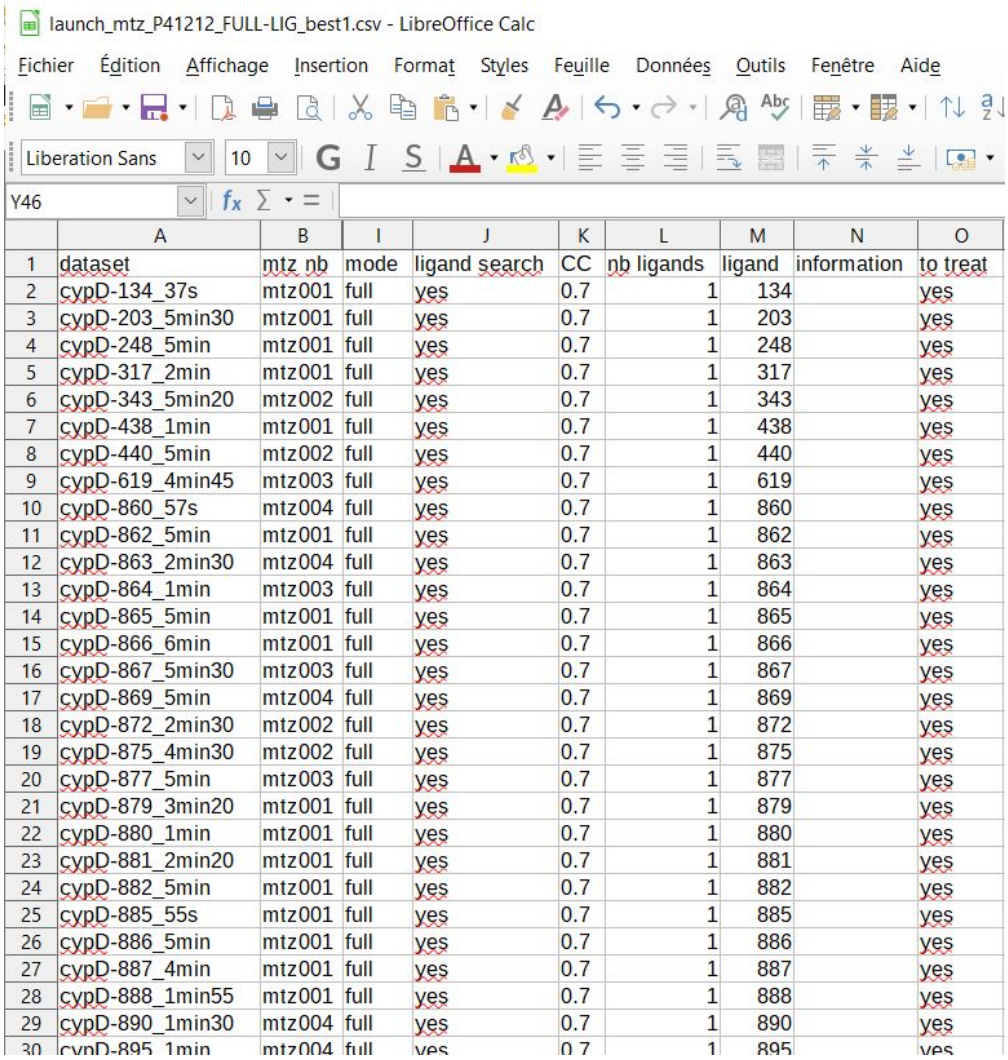
W44

	A	B	I	J	K	L	M	N	O
1	dataset	mtz nb	mode	ligand search	CC	nb ligands	ligand	information	to treat
2	cypD-134_37s	mtz001	allsg	no					yes
3	cypD-172_1min20	mtz003	allsg	no					yes
4	cypD-203_5min30	mtz001	allsg	no					yes
5	cypD-248_5min	mtz001	allsg	no					yes
6	cypD-317_2min	mtz001	allsg	no					yes
7	cypD-343_5min20	mtz002	allsg	no					yes
8	cypD-438_1min	mtz001	allsg	no					yes
9	cypD-440_5min	mtz001	allsg	no					yes
10	cypD-619_4min45	mtz003	allsg	no					yes
11	cypD-860_57s	mtz004	allsg	no					yes
12	cypD-861_5min30	mtz001	fast	no				resolution > 3.75A	yes
13	cypD-862_5min	mtz001	allsg	no					yes
14	cypD-863_2min30	mtz004	allsg	no					yes
15	cypD-864_1min	mtz003	allsg	no					yes
16	cypD-865_5min	mtz001	allsg	no					yes
17	cypD-866_6min	mtz001	allsg	no					yes
18	cypD-867_5min30	mtz003	allsg	no					yes
19	cypD-869_5min	mtz004	allsg	no					yes
20	cypD-872_2min30	mtz002	allsg	no					yes
21	cypD-874_5min30	mtz001	allsg	no					yes
22	cypD-875_4min30	mtz002	allsg	no					yes
23	cypD-877_5min	mtz003	allsg	no					yes
24	cypD-878_5min	mtz002	allsg	no					yes
25	cypD-879_3min20	mtz001	allsg	no					yes
26	cypD-880_1min	mtz001	allsg	no					yes
27	cypD-881_2min20	mtz001	allsg	no					yes
28	cypD-882_5min	mtz001	allsg	no					yes
29	cypD-884_5min	mtz002	allsg	no					yes
30	cypD-885_55s	mtz001	allsg	no					yes
31	cypD-886_5min	mtz001	allsg	no					yes
32	cypD-887_4min	mtz001	allsg	no					yes
33	cypD-888_1min55	mtz001	allsg	no					yes
34	cypD-889_2min	mtz001	allsg	no					yes

- Option example: –mode full –lig

Phenix will be run in 'full' mode. Then ligand will be searched with LigandFit[2] and placed if cutoff model-to-map CC is more than 0.7 (default). This cutoff can be changed with '–cclig' option. The number of ligands to be placed (default=1) can be changed with '–nblig' option.

[2] https://www.phenix-online.org/documentation/reference/ligandfit.html


launch_mtz_P41212_FULL-LIG_best1.csv - LibreOffice Calc

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Liberation Sans 10

Y46

	A	B	I	J	K	L	M	N	O
1	dataset	mtz nb	mode	ligand search	CC	nb ligands	ligand	information	to treat
2	cypD-134_37s	mtz001	full	yes	0.7	1	134		yes
3	cypD-203_5min30	mtz001	full	yes	0.7	1	203		yes
4	cypD-248_5min	mtz001	full	yes	0.7	1	248		yes
5	cypD-317_2min	mtz001	full	yes	0.7	1	317		yes
6	cypD-343_5min20	mtz002	full	yes	0.7	1	343		yes
7	cypD-438_1min	mtz001	full	yes	0.7	1	438		yes
8	cypD-440_5min	mtz002	full	yes	0.7	1	440		yes
9	cypD-619_4min45	mtz003	full	yes	0.7	1	619		yes
10	cypD-860_57s	mtz004	full	yes	0.7	1	860		yes
11	cypD-862_5min	mtz001	full	yes	0.7	1	862		yes
12	cypD-863_2min30	mtz004	full	yes	0.7	1	863		yes
13	cypD-864_1min	mtz003	full	yes	0.7	1	864		yes
14	cypD-865_5min	mtz001	full	yes	0.7	1	865		yes
15	cypD-866_6min	mtz001	full	yes	0.7	1	866		yes
16	cypD-867_5min30	mtz003	full	yes	0.7	1	867		yes
17	cypD-869_5min	mtz004	full	yes	0.7	1	869		yes
18	cypD-872_2min30	mtz002	full	yes	0.7	1	872		yes
19	cypD-875_4min30	mtz002	full	yes	0.7	1	875		yes
20	cypD-877_5min	mtz003	full	yes	0.7	1	877		yes
21	cypD-879_3min20	mtz001	full	yes	0.7	1	879		yes
22	cypD-880_1min	mtz001	full	yes	0.7	1	880		yes
23	cypD-881_2min20	mtz001	full	yes	0.7	1	881		yes
24	cypD-882_5min	mtz001	full	yes	0.7	1	882		yes
25	cypD-885_55s	mtz001	full	yes	0.7	1	885		yes
26	cypD-886_5min	mtz001	full	yes	0.7	1	886		yes
27	cypD-887_4min	mtz001	full	yes	0.7	1	887		yes
28	cypD-888_1min55	mtz001	full	yes	0.7	1	888		yes
29	cypD-890_1min30	mtz004	full	yes	0.7	1	890		yes
30	cypD-895_1min	mtz004	full	yes	0.7	1	895		yes

9.2.4 4. Launch Phenix according to chosen mode and options

phenix.ligand_pipeline[1] is launched for each mtz file according to chosen mode and options, as listed in the 'launch csv' file (see 3. above).

If this 'launch csv' exists and you have modified something like adding a ligand cif for example, 'launch' mode should be run again, but in simulation mode so as it generates a new correct launch csv file instead of using existing one. When a new 'launch csv' file has been generated, just run the same command without simulation mode.

Example:

```
$ easypipe.py PROCESSED_DATA launch my_ref_folder --mode full --lig --autoproc --
↪simulate
then:
$ easypipe.py PROCESSED_DATA launch my_ref_folder --mode full --lig --autoproc
```

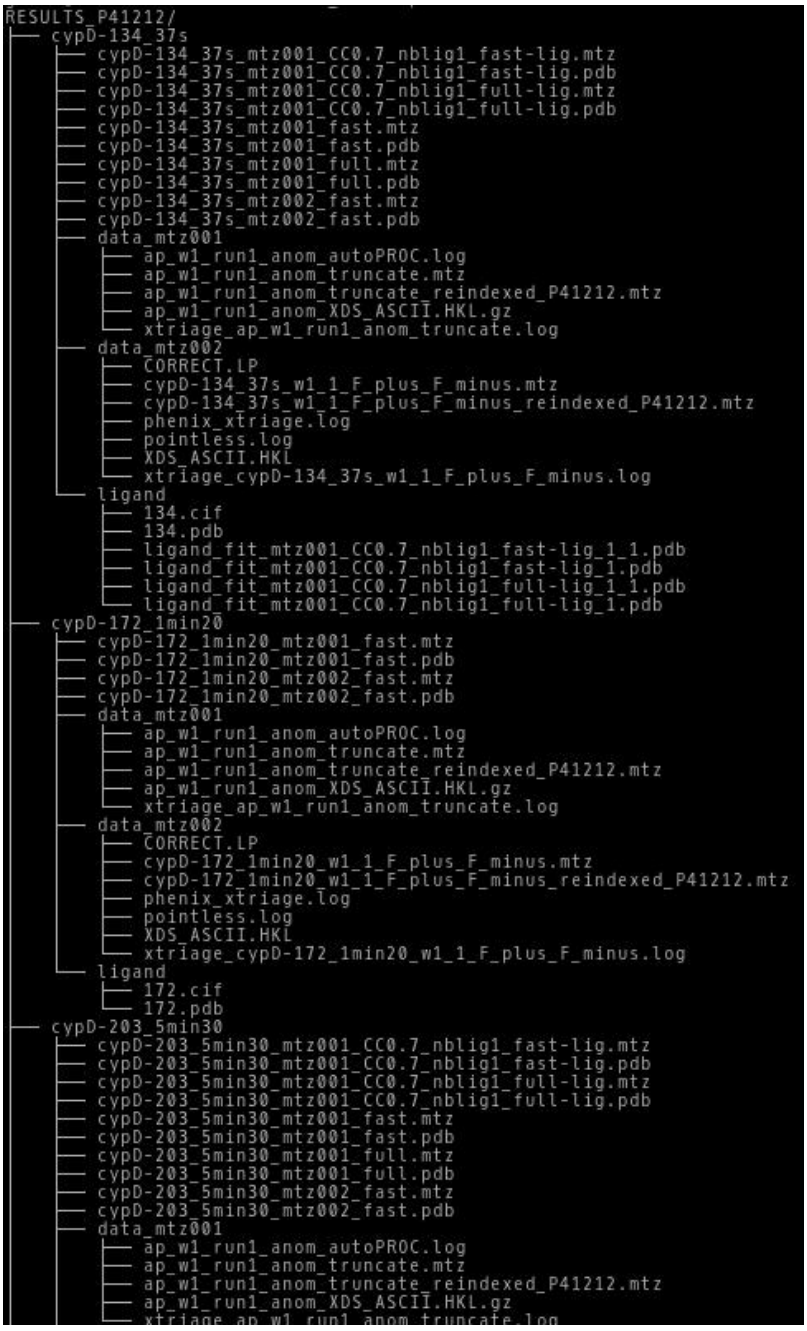
Simulation mode also allows to modify the 'to treat' column of the 'launch csv' file (replacing 'yes' by 'no'). Useful if you want to run some options only on some mtz. Then just run the same command without simulation mode. You can also modify the following columns: 'mode', 'ligand search', 'CC', 'nb ligands', as long as you know what you are doing.

9.2.5 5. Write results

At the end of each 'launch' subcommand, results are copied in a 'RESULT' folder.

In datasets folders, copy of:

- corresponding processed data and logs (useful for deposition at the PDB)
- pdb and mtz result files
- phenix cif file if ligand found
- ligand folder, if exists
- pdb of ligand(s) placed by LigandFit (all CC)



In a '_mtz_treated' folder, copy of:

- csv listing datasets without mtz file
- csv with mtz list
- csv with mtz list after reindexing
- csv with mtz list sorted according to reference space group
- all 'launch' csv files, with a counter at the end of the names in case of several launches (with handmade modifications of launch csv file for example)

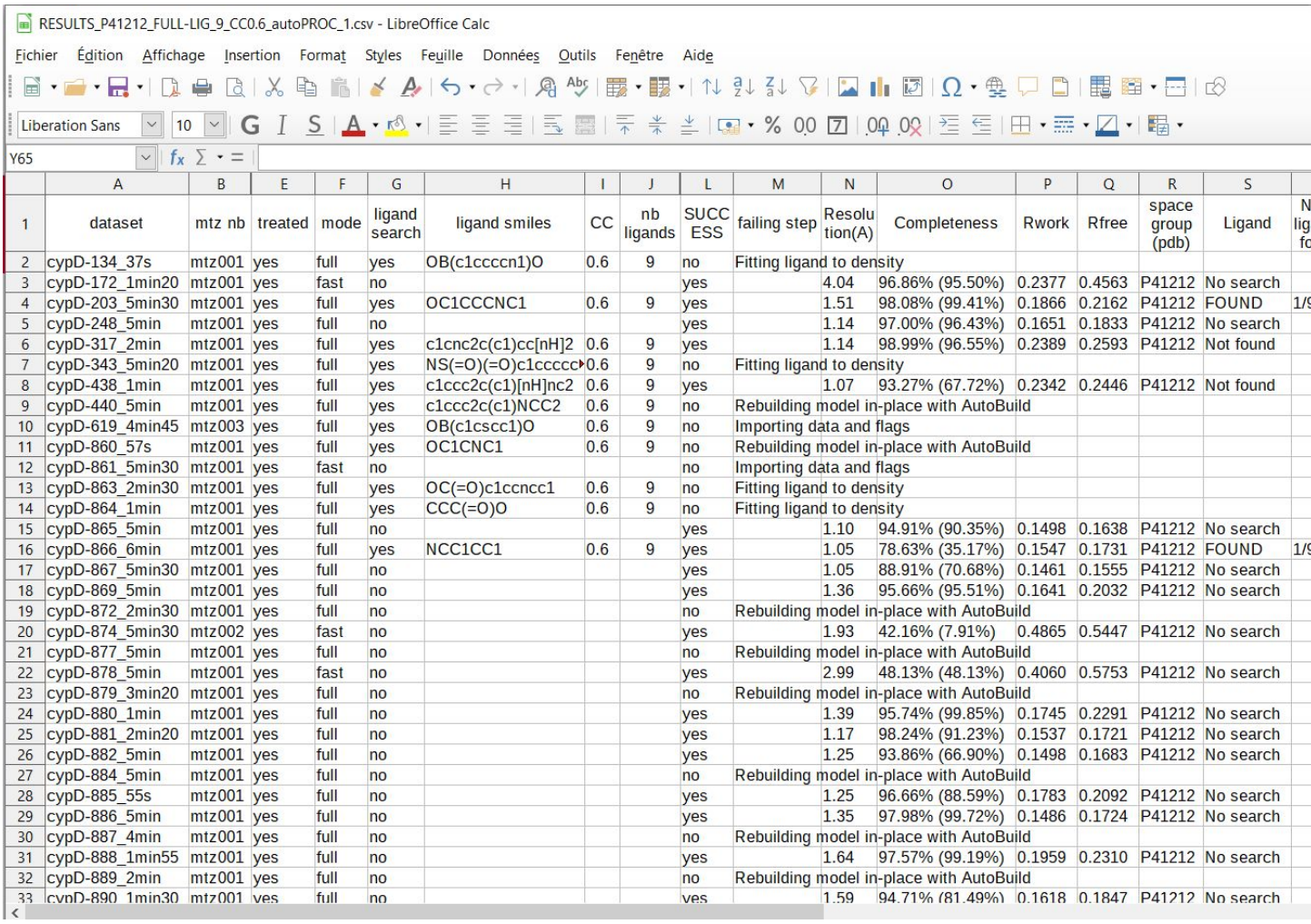
```
mtz_treated/
├── launch_mtz_P41212_FAST_autoPROC_1.csv
├── launch_mtz_P41212_FAST_best1_1.csv
├── launch_mtz_P41212_FAST_best2_1.csv
├── launch_mtz_P41212_FAST-LIG_best1_1.csv
├── launch_mtz_P41212_FAST-LIG_best1_2.csv
├── launch_mtz_P41212_FULL_autoPROC_1.csv
├── launch_mtz_P41212_FULL_best1_1.csv
├── launch_mtz_P41212_FULL-LIG_9_CC0.6_autoPROC_1.csv
├── launch_mtz_P41212_FULL-LIG_9_CC0.6_autoPROC_2.csv
├── launch_mtz_P41212_FULL-LIG_9_CC0.6_autoPROC_3.csv
├── launch_mtz_P41212_FULL-LIG_9_CC0.6_best1_1.csv
├── launch_mtz_P41212_FULL-LIG_9_CC0.6_best1_2.csv
├── launch_mtz_P41212_FULL-LIG_best1_1.csv
├── launch_mtz_P41212_FULL-LIG_best1_2.csv
├── mtz_to_treat_ALL.csv
├── mtz_to_treat_ALL_reindexed.csv
└── mtz_to_treat_ALL_reindexed_sorted_P41212.csv
```

For each 'launch' subcommand, a csv file is created that summarizes the corresponding results for each dataset, with information on:

- success of Phenix
- failing step (in case success = no)
- resolution
- completeness
- Rwork / Rfree
- space group
- if ligand has been placed, number of ligands found, corresponding CC

```
├── RESULTS_P41212_FAST_autoPROC_1.csv
├── RESULTS_P41212_FAST_best1_1.csv
├── RESULTS_P41212_FAST_best2_1.csv
├── RESULTS_P41212_FAST-LIG_best1_1.csv
├── RESULTS_P41212_FAST-LIG_best1_2.csv
├── RESULTS_P41212_FULL_autoPROC_1.csv
├── RESULTS_P41212_FULL_best1_1.csv
├── RESULTS_P41212_FULL-LIG_9_CC0.6_autoPROC_1.csv
├── RESULTS_P41212_FULL-LIG_9_CC0.6_autoPROC_2.csv
├── RESULTS_P41212_FULL-LIG_9_CC0.6_autoPROC_3.csv
├── RESULTS_P41212_FULL-LIG_9_CC0.6_best1_1.csv
├── RESULTS_P41212_FULL-LIG_9_CC0.6_best1_2.csv
├── RESULTS_P41212_FULL-LIG_best1_1.csv
├── RESULTS_P41212_FULL-LIG_best1_2.csv
```

Option example: -a –mode full –lig –nblig 9 –cclig 0.6


RESULTS_P41212_FULL-LIG_9_CC0.6_autoPROC_1.csv - LibreOffice Calc

Fichier Édition Affichage Insertion Format Styles Feuille Données Outils Fenêtre Aide

Liberation Sans 10

Y65

	A	B	E	F	G	H	I	J	L	M	N	O	P	Q	R	S	
1	dataset	mtz nb	treated	mode	ligand search	ligand smiles	CC	nb ligands	SUCCESS	failing step	Resolution(A)	Completeness	Rwork	Rfree	space group (pdb)	Ligand	N lig fo
2	cypD-134_37s	mtz001	yes	full	yes	OB(c1ccccn1)O	0.6	9	no	Fitting ligand to density							
3	cypD-172_1min20	mtz001	yes	fast	no				yes		4.04	96.86% (95.50%)	0.2377	0.4563	P41212	No search	
4	cypD-203_5min30	mtz001	yes	full	yes	OC1CCCNC1	0.6	9	yes		1.51	98.08% (99.41%)	0.1866	0.2162	P41212	FOUND	1/9
5	cypD-248_5min	mtz001	yes	full	no				yes		1.14	97.00% (96.43%)	0.1651	0.1833	P41212	No search	
6	cypD-317_2min	mtz001	yes	full	yes	c1cnc2c(c1)cc[nH]2	0.6	9	yes		1.14	98.99% (96.55%)	0.2389	0.2593	P41212	Not found	
7	cypD-343_5min20	mtz001	yes	full	yes	NS(=O)(=O)c1ccccc	0.6	9	no	Fitting ligand to density							
8	cypD-438_1min	mtz001	yes	full	yes	c1ccc2c(c1)[nH]nc2	0.6	9	yes		1.07	93.27% (67.72%)	0.2342	0.2446	P41212	Not found	
9	cypD-440_5min	mtz001	yes	full	yes	c1ccc2c(c1)NCC2	0.6	9	no	Rebuilding model in-place with AutoBuild							
10	cypD-619_4min45	mtz003	yes	full	yes	OB(c1cscc1)O	0.6	9	no	Importing data and flags							
11	cypD-860_57s	mtz001	yes	full	yes	OC1CNC1	0.6	9	no	Rebuilding model in-place with AutoBuild							
12	cypD-861_5min30	mtz001	yes	fast	no				no	Importing data and flags							
13	cypD-863_2min30	mtz001	yes	full	yes	OC(=O)c1ccncc1	0.6	9	no	Fitting ligand to density							
14	cypD-864_1min	mtz001	yes	full	yes	CCC(=O)O	0.6	9	no	Fitting ligand to density							
15	cypD-865_5min	mtz001	yes	full	no				yes		1.10	94.91% (90.35%)	0.1498	0.1638	P41212	No search	
16	cypD-866_6min	mtz001	yes	full	yes	NCC1CC1	0.6	9	yes		1.05	78.63% (35.17%)	0.1547	0.1731	P41212	FOUND	1/9
17	cypD-867_5min30	mtz001	yes	full	no				yes		1.05	88.91% (70.68%)	0.1461	0.1555	P41212	No search	
18	cypD-869_5min	mtz001	yes	full	no				yes		1.36	95.66% (95.51%)	0.1641	0.2032	P41212	No search	
19	cypD-872_2min30	mtz001	yes	full	no				no	Rebuilding model in-place with AutoBuild							
20	cypD-874_5min30	mtz002	yes	fast	no				yes		1.93	42.16% (7.91%)	0.4865	0.5447	P41212	No search	
21	cypD-877_5min	mtz001	yes	full	no				no	Rebuilding model in-place with AutoBuild							
22	cypD-878_5min	mtz001	yes	fast	no				yes		2.99	48.13% (48.13%)	0.4060	0.5753	P41212	No search	
23	cypD-879_3min20	mtz001	yes	full	no				no	Rebuilding model in-place with AutoBuild							
24	cypD-880_1min	mtz001	yes	full	no				yes		1.39	95.74% (99.85%)	0.1745	0.2291	P41212	No search	
25	cypD-881_2min20	mtz001	yes	full	no				yes		1.17	98.24% (91.23%)	0.1537	0.1721	P41212	No search	
26	cypD-882_5min	mtz001	yes	full	no				yes		1.25	93.86% (66.90%)	0.1498	0.1683	P41212	No search	
27	cypD-884_5min	mtz001	yes	full	no				no	Rebuilding model in-place with AutoBuild							
28	cypD-885_55s	mtz001	yes	full	no				yes		1.25	96.66% (88.59%)	0.1783	0.2092	P41212	No search	
29	cypD-886_5min	mtz001	yes	full	no				yes		1.35	97.98% (99.72%)	0.1486	0.1724	P41212	No search	
30	cypD-887_4min	mtz001	yes	full	no				no	Rebuilding model in-place with AutoBuild							
31	cypD-888_1min55	mtz001	yes	full	no				yes		1.64	97.57% (99.19%)	0.1959	0.2310	P41212	No search	
32	cypD-889_2min	mtz001	yes	full	no				no	Rebuilding model in-place with AutoBuild							
33	cypD-890_1min30	mtz001	yes	full	no				yes		1.59	94.71% (81.49%)	0.1618	0.1847	P41212	No search	

Note: To compile the results of all 'launch' subcommands you have run, run *'summary'* subcommand

9.3 Phenix options according to modes (only for information)

phenix.ligand_pipeline[1] options are the following:

- common options:

nproc=Auto

preserve_chain_id=True: Preserves the original chain ID

refine.after_ligand.hydrogens=False: Hydrogen atoms won't be added prior to the final refinement step (else refinement significantly slower)

prune=False: disable Prune the model after refinement to remove residues and sidechains in poor density

keep_hetatms=True: prevent Phaser from resetting HETATMs occupancies to zero

refine.after_mr.update_waters=False: don't add/remove waters automatically

- 'fast' mode:

skip_xtriage=True

mr=False: rigid-body refinement will be used

quick_refine=True: which will shorten both refinement steps from 6 to 3 cycles, and disable weight optimization.

build=False

skip_ligand=True

reference_structure='model.pdb': If specified, phenix.find_alt_orig_sym_mate will be applied to map the solution to the reference structure (not working when Phaser with several monomers)

- 'full' mode:

mr=Auto: the program will try rigid-body refinement first, then run Phaser if the R-free is too high (>0.4)

build=Auto: Run AutoBuild after initial refinement. By default, this will be done if R-free is greater than the max_r_free cutoff = 0.3

autobuild.quick=True: Run AutoBuild in quick mode. Inferior results, but a huge time-saver

quick_refine=True: which will shorten both refinement steps from 6 to 3 cycles, and disable weight optimization.

- 'allsg' mode:

mr=True

quick_refine=False

- if ligand search:

ligand_copies=1 (except if option –nblig >1)

keep_input_restraints=True : if the input files include pre-calculated restraints for the target ligand, eLBOW will propagate these restraints instead of generating new ones.

9.4 References

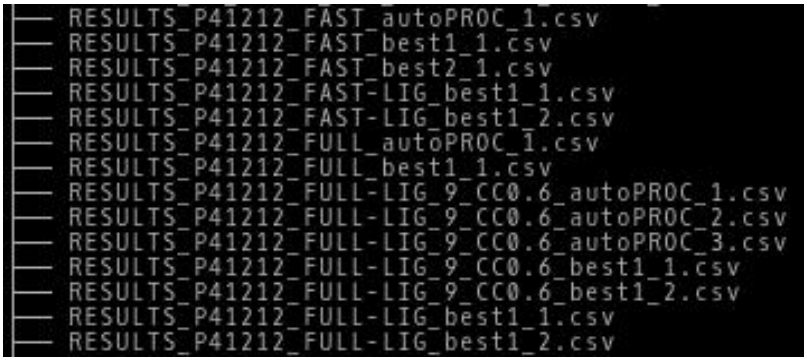
CHAPTER

TEN

EASYPIPE 'SUMMARY'

This step can be run after several runs of *'launch'* subcommands.

For each 'launch' subcommand, a 'RESULT' csv file is created that summarizes the corresponding results for each dataset (*see here*). So, if you have tried several options, you will have as many 'RESULTS' csv files.



Then, you probably want to compile all these results for a better view.

10.1 Usage

easypipe.py data summary [-h]

Example:

```
$ easypipe.py PROCESSED_DATA summary
```

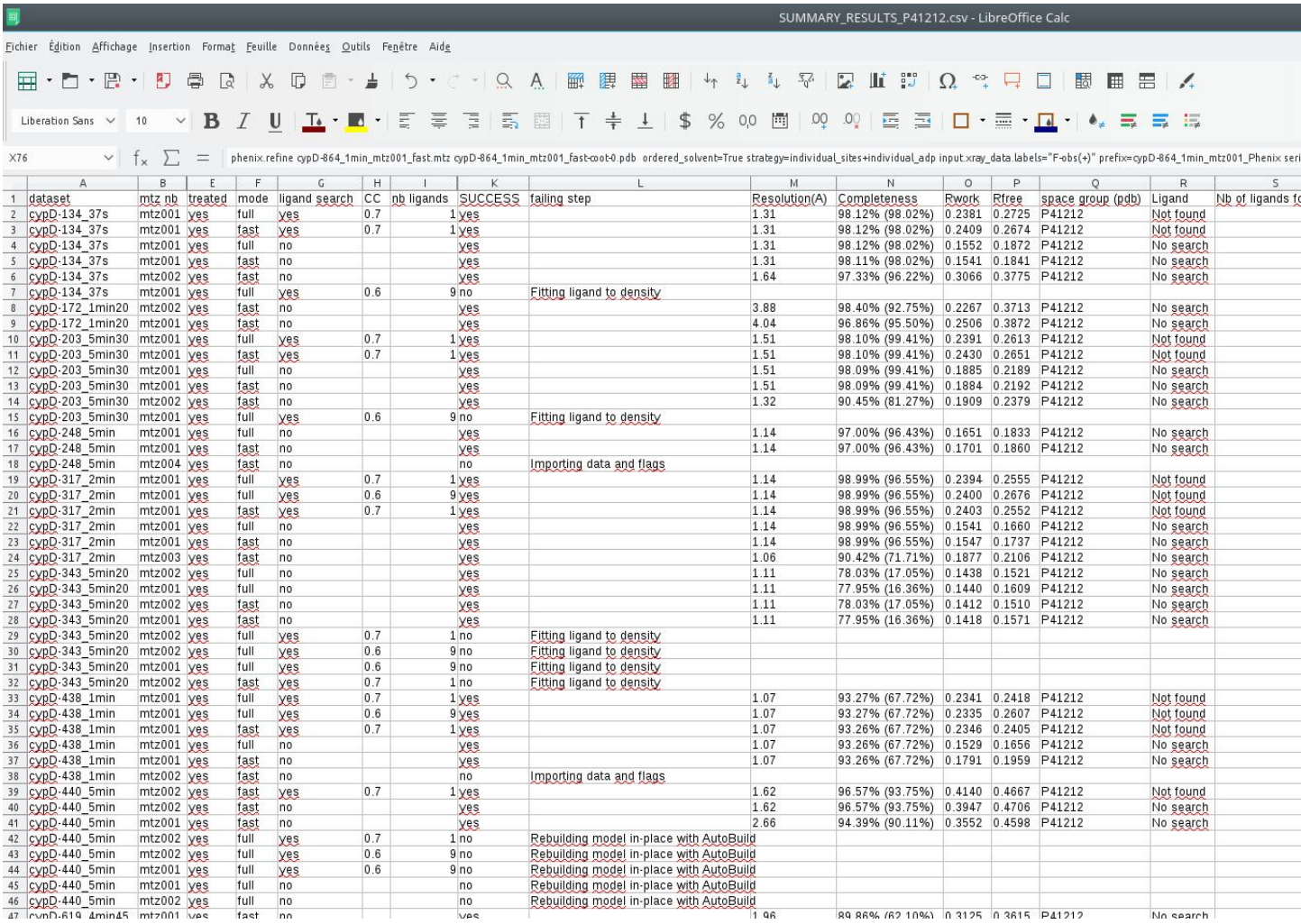
10.2 What does it do ?

In the 'RESULT' folder, 'summary' creates a 'SUMMARY' csv file where all datasets results are compiled.

For each datasets, redondant results are deleted and the remaining ones are sorted according to:

- 'dataset'
- 'SUCCESS'
- 'ligand search'
- 'mode'
- 'Ligand' (found or not)

- 'Completeness'



	A	B	E	F	G	H	I	K	L	M	N	O	P	Q	R	S
1	dataset	mtz nb	treated	mode	ligand search	CC	nb ligands	SUCCESS	failing step	Resolution(A)	Completeness	Rwork	Rfree	space group (pdb)	Ligand	Nb of ligands fo
2	cypD-134_37s	mtz001	yes	full	yes	0.7	1	yes		1.31	98.12% (98.02%)	0.2381	0.2725	P41212	Not found	
3	cypD-134_37s	mtz001	yes	fast	yes	0.7	1	yes		1.31	98.12% (98.02%)	0.2409	0.2674	P41212	Not found	
4	cypD-134_37s	mtz001	yes	full	no			yes		1.31	98.12% (98.02%)	0.1552	0.1872	P41212	No search	
5	cypD-134_37s	mtz001	yes	fast	no			yes		1.31	98.11% (98.02%)	0.1541	0.1841	P41212	No search	
6	cypD-134_37s	mtz002	yes	fast	no			yes		1.64	97.33% (96.22%)	0.3066	0.3775	P41212	No search	
7	cypD-134_37s	mtz001	yes	full	yes	0.6	9	no	Fitting ligand to density							
8	cypD-172_1min20	mtz002	yes	fast	no			yes		3.88	98.40% (92.75%)	0.2267	0.3713	P41212	No search	
9	cypD-172_1min20	mtz001	yes	fast	no			yes		4.04	96.86% (95.50%)	0.2506	0.3872	P41212	No search	
10	cypD-203_5min30	mtz001	yes	full	yes	0.7	1	yes		1.51	98.10% (99.41%)	0.2391	0.2613	P41212	Not found	
11	cypD-203_5min30	mtz001	yes	fast	yes	0.7	1	yes		1.51	98.10% (99.41%)	0.2430	0.2651	P41212	Not found	
12	cypD-203_5min30	mtz001	yes	full	no			yes		1.51	98.09% (99.41%)	0.1885	0.2189	P41212	No search	
13	cypD-203_5min30	mtz001	yes	fast	no			yes		1.51	98.09% (99.41%)	0.1884	0.2192	P41212	No search	
14	cypD-203_5min30	mtz002	yes	fast	no			yes		1.32	90.45% (81.27%)	0.1909	0.2379	P41212	No search	
15	cypD-203_5min30	mtz001	yes	full	yes	0.6	9	no	Fitting ligand to density							
16	cypD-248_5min	mtz001	yes	full	no			yes		1.14	97.00% (96.43%)	0.1651	0.1833	P41212	No search	
17	cypD-248_5min	mtz001	yes	fast	no			yes		1.14	97.00% (96.43%)	0.1701	0.1860	P41212	No search	
18	cypD-248_5min	mtz004	yes	fast	no			no	Importing data and flags							
19	cypD-317_2min	mtz001	yes	full	yes	0.7	1	yes		1.14	98.99% (96.55%)	0.2394	0.2555	P41212	Not found	
20	cypD-317_2min	mtz001	yes	full	yes	0.6	9	yes		1.14	98.99% (96.55%)	0.2400	0.2676	P41212	Not found	
21	cypD-317_2min	mtz001	yes	fast	yes	0.7	1	yes		1.14	98.99% (96.55%)	0.2403	0.2552	P41212	Not found	
22	cypD-317_2min	mtz001	yes	full	no			yes		1.14	98.99% (96.55%)	0.1541	0.1660	P41212	No search	
23	cypD-317_2min	mtz001	yes	fast	no			yes		1.14	98.99% (96.55%)	0.1547	0.1737	P41212	No search	
24	cypD-317_2min	mtz003	yes	fast	no			yes		1.06	90.42% (71.71%)	0.1877	0.2106	P41212	No search	
25	cypD-343_5min20	mtz002	yes	full	no			yes		1.11	78.03% (17.05%)	0.1438	0.1521	P41212	No search	
26	cypD-343_5min20	mtz001	yes	full	no			yes		1.11	77.95% (16.36%)	0.1440	0.1609	P41212	No search	
27	cypD-343_5min20	mtz002	yes	fast	no			yes		1.11	78.03% (17.05%)	0.1412	0.1510	P41212	No search	
28	cypD-343_5min20	mtz001	yes	fast	no			yes		1.11	77.95% (16.36%)	0.1418	0.1571	P41212	No search	
29	cypD-343_5min20	mtz002	yes	full	yes	0.7	1	no	Fitting ligand to density							
30	cypD-343_5min20	mtz002	yes	full	yes	0.6	9	no	Fitting ligand to density							
31	cypD-343_5min20	mtz001	yes	full	yes	0.6	9	no	Fitting ligand to density							
32	cypD-343_5min20	mtz002	yes	fast	yes	0.7	1	no	Fitting ligand to density							
33	cypD-438_1min	mtz001	yes	full	yes	0.7	1	yes		1.07	93.27% (67.72%)	0.2341	0.2418	P41212	Not found	
34	cypD-438_1min	mtz001	yes	full	yes	0.6	9	yes		1.07	93.27% (67.72%)	0.2335	0.2607	P41212	Not found	
35	cypD-438_1min	mtz001	yes	fast	yes	0.7	1	yes		1.07	93.26% (67.72%)	0.2346	0.2405	P41212	Not found	
36	cypD-438_1min	mtz001	yes	full	no			yes		1.07	93.26% (67.72%)	0.1529	0.1656	P41212	No search	
37	cypD-438_1min	mtz001	yes	fast	no			yes		1.07	93.26% (67.72%)	0.1791	0.1959	P41212	No search	
38	cypD-438_1min	mtz002	yes	fast	no			no	Importing data and flags							
39	cypD-440_5min	mtz002	yes	fast	yes	0.7	1	yes		1.62	96.57% (93.75%)	0.4140	0.4667	P41212	Not found	
40	cypD-440_5min	mtz002	yes	fast	no			yes		1.62	96.57% (93.75%)	0.3947	0.4706	P41212	No search	
41	cypD-440_5min	mtz001	yes	fast	no			yes		2.66	94.39% (90.11%)	0.3552	0.4598	P41212	No search	
42	cypD-440_5min	mtz002	yes	full	yes	0.7	1	no	Rebuilding model in-place with AutoBuild							
43	cypD-440_5min	mtz002	yes	full	yes	0.6	9	no	Rebuilding model in-place with AutoBuild							
44	cypD-440_5min	mtz001	yes	full	yes	0.6	9	no	Rebuilding model in-place with AutoBuild							
45	cypD-440_5min	mtz001	yes	full	no			no	Rebuilding model in-place with AutoBuild							
46	cypD-440_5min	mtz002	yes	full	no			no	Rebuilding model in-place with AutoBuild							
47	cypD-619_4min45	mtz001	yes	fast	no			yes		1.96	89.86% (62.10%)	0.3125	0.3615	P41212	No search	

This way, the first row of each dataset should be most of the time the best treatment to consider, but is always better to have a critical eye on information like completeness or resolution to be sure …

CHAPTER

ELEVEN

EASYPIPE 'AUTO'

This mode allows to launch main easYPipe steps (prep, reindex, launch, summary) without any intervention. Ligand search is not possible for the moment.

11.1 Usage

easypipe.py data auto [-h] [-m {fast,full,allsg}] ref

arguments	description
ref	folder with fasta file and pdb file for replacement, and cif(s) if ligand(s) in the model

Warning: reference pdb files should include the row starting with 'CRYST1' containing information on space group

optional arguments	description
-h, –help	show this help message and exit
-m {fast,full,allsg}, –mode {fast,full,allsg}	running mode: fast, full, or allsg (default = fast)
-b NUMBER, –best NUMBER	launch only for mtz with best completeness, NUMBER indicates how many mtz to treat (default 1), ex: –best 2
-a, –autoproc	launch only for mtz from autoPROC, or if none launch for mtz with best completeness
-w, –whole	launch for the whole mtz processes
-t TEMPLATE, –template TEMPLATE	optional template name for log files and result folders, in case re-launching with different reference pdb of the same space group (else will overwrite).

Example:

```
$ easypipe.py PROCESSED_DATA auto my_ref_folder --best 2 --mode full
equivalent to:
$ easypipe.py PROCESSED_DATA auto my_ref_folder -b 2 -m full
```

11.2 How the data should be organized ?

Processed data should be in datasets folders, all grouped in a folder. More information on how to organize your data *here*.

11.3 What does it do ?

Executes successively, without any intervention, the following steps:

- *prep*
- *reindex*
- *launch*
- *summary*

The options are the same as for *launch*, except for the options concerning the search for ligands which is not enabled at the moment. In the same way, the option "simulate" is not possible because it would imply an intervention. A new 'launch csv' file is therefore generated each time.

CHAPTER

TWELVE

EASYPIPE 'PANDDA'

If you have more than 40 datasets, you can try to use PanDDA[1] which is particularly suitable to the detection of weakly bound ligands such as fragments.

This step can be run after all 'launch' subcommands have been executed, and aims at organizing the data processed with easYPipe in order to be able to run PanDDA.

12.1 Usage

easypipe.py data pandda [-h]

Example:

```
$ easypipe.py ./PROCESSED_DATA/ pandda
```

12.2 What does it do ?

For each dataset, 'pandda' easYPipe subcommand copies in a dataset folder suitable for PanDDA:

- pdb and mtz files generated with easYPipe,
- cif and pdb files of corresponding ligand,

[1] https://pandda.bitbucket.io/

```
PANDDA/
├── logs
│   └── pandda-data_easypipe_2021-02-24_195235.log
└── PANDDA_P41212
    └── data
        ├── cypD-134_37s_mtz001
        │   ├── 134.cif
        │   ├── 134.pdb
        │   ├── cypD-134_37s_mtz001_full.mtz
        │   └── cypD-134_37s_mtz001_full.pdb
        ├── cypD-203_5min30_mtz001
        │   ├── 203.cif
        │   ├── 203.pdb
        │   ├── cypD-203_5min30_mtz001_full.mtz
        │   └── cypD-203_5min30_mtz001_full.pdb
        ├── cypD-248_5min_mtz001
        │   ├── 248.cif
        │   ├── 248.pdb
        │   ├── cypD-248_5min_mtz001_full.mtz
        │   └── cypD-248_5min_mtz001_full.pdb
        ├── cypD-317_2min_mtz001
        │   ├── 317.cif
        │   ├── 317.pdb
        │   ├── cypD-317_2min_mtz001_full.mtz
        │   └── cypD-317_2min_mtz001_full.pdb
        ├── cypD-343_5min20_mtz002
        │   ├── 343.cif
        │   ├── 343.pdb
        │   ├── cypD-343_5min20_mtz002_full.mtz
        │   └── cypD-343_5min20_mtz002_full.pdb
        ├── cypD-438_1min_mtz001
        │   ├── 438.cif
        │   ├── 438.pdb
        │   ├── cypD-438_1min_mtz001_full.mtz
        │   └── cypD-438_1min_mtz001_full.pdb
        ├── cypD-440_5min_mtz002
        │   ├── 440.cif
        │   ├── 440.pdb
        │   ├── cypD-440_5min_mtz002_fast.mtz
        │   └── cypD-440_5min_mtz002_fast.pdb
        ├── cypD-619_4min45_mtz003
        │   ├── 619.cif
```

12.3 References